ONR BAA Announcement Number : 10-026



## **BROAD AGENCY ANNOUNCEMENT (BAA)**

#### **INTRODUCTION:**

This publication constitutes a Broad Agency Announcement (BAA) as contemplated in Department of Defense Grant and Agreement Regulation (DODGARS) 22.315(a). A formal Request for Proposals (RFP), solicitation, and/or additional information regarding this announcement will not be issued. Request for same will be disregarded.

The Office of Naval Research (ONR) will not issue paper copies of this announcement. The ONR and Department of Defense (DoD) agencies involved in this program reserve the right to select for award all, some or none of the proposals submitted in response to this announcement. The ONR and other participating DoD agencies provide no funding for direct reimbursement of proposal development costs. Technical and cost proposals (or any other material) submitted in response to this BAA will not be returned. It is the policy of ONR and participating DoD agencies to treat all proposals as sensitive competitive information and to disclose their contents only for the purposes of evaluation.

The DoD Multidisciplinary University Research Initiative (MURI), one element of the University Research Initiative (URI), is sponsored by the DoD research offices: the Office of Naval Research (ONR), the Army Research Office (ARO), and the Air Force Office of Scientific Research (AFOSR) (hereafter collectively referred to as "DoD agencies").

Awards will take the form of grants. Therefore, proposals submitted as a result of this announcement will fall under the purview of the Department of Defense Grant and Agreement Regulations (DoDGARs).

Potential offerors may obtain information on ONR programs and opportunities by checking the ONR website at http://www.onr.navy.mil/en/Contracts-Grants/Funding-Opportunities/Broad-Agency-Announcements.aspx.

# I. GENERAL INFORMATION

### 1. Agency Name

Office of Naval Research 875 North Randolph Street - Suite 1425 Code 03R Arlington, VA 22203-1995

# 2. Research Opportunity Title

Multidisciplinary University Research Initiative (MURI)

#### 3. Program Name

Fiscal Year (FY) 2011 Department of Defense Multidisciplinary Research Program of the University Research Initiative

# 4. Research Opportunity Number

BAA 10-026

### 5. Response Date

White Papers: Thursday, 30 September 2010

Full Proposals: Tuesday, 07 December 2010

### 6. Research Opportunity Description

Synopsis

The MURI program supports basic science and/or engineering research at U.S. institutions of higher education (hereafter referred to as "universities") that is of potential interest to DoD. The program is focused on multidisciplinary research efforts that intersect more than one traditional science and engineering discipline to address scientific issues of interest to the DoD. As defined by the DoD, "basic research is systematic study directed toward greater knowledge or understanding of the fundamental aspects of phenomena and of observable facts without specific applications towards processes or products in mind. It includes all scientific study and experimentation directed toward increasing fundamental knowledge and understanding in those fields of the physical, engineering, environmental, and life sciences related to long-term national security needs. It is farsighted high payoff research that provides the basis for technological progress." (http://comptroller.defense.gov/fmr/02b/02b\_05.pdf). The DoD's basic research program invests broadly in many specific fields to ensure that it has early cognizance of new scientific knowledge.

The FY 2011 MURI competition is for the topics listed below. Detailed descriptions of the topics can be found in Section VIII entitled, "Specific MURI Topics", of this BAA. The detailed descriptions are intended to provide the proposer a frame of reference and are not meant to be restrictive to the possible approaches to achieving the goals of the topic and the program. Innovative ideas addressing these research topics are highly encouraged.

White papers and full proposals addressing the following topics (1) through (10) should be submitted to The Office of Naval Research:

- (1) Soil Blast Modeling and Simulation
- (2) Knowledge Representation and Reasoning for Decentralized Autonomy
- (3) III-Nitride Terahertz Electronics Scaling Strategies beyond Silicon
- (4) Charge Transport in DNA Molecular Wire
- (5) Coupled Human-landscape Interactions in Low-lying Coastal Environments
- (6) Integrated Oceanographic, Atmospheric, and Acoustic Physics
- (7) Improved Meteorlogical Modeling in Mountainous Terrain
- (8) Bacterial or Cellular Controllers for Device Autonomy
- (9) Nanoscience based High-speed Fabrication of Full Function Hybrid Flexible Electronic Systems
- (10) Atomic-scale Interphases: Exploring New Material States

White papers and Full proposals addressing the following topics (11) through (17) should be submitted to the Air Force Office of Scientific Research (AFOSR):

- (11) Nanofabrication of Tunable 3D Nanotube Architectures (2 proposals)
- (12) Quantum Memories and Light-Matter Interfaces (2 proposals)
- (13) Biomolecule-Directed Assembly of Nanostructures
- (14) Nanostructural Control of Thermal and Electrical Transport Properties
- (15) Investigation of 3-D Hybrid Integration of CMOS/Nanoelectronic Circuits
- (16) Science of Cyber Security
- (17) Large Scale Integrated Hybrid Nanophotonics

White papers and full proposals addressing the following topics (18) through (25) should be submitted to the Army Research Office (ARO):

- (18) Controlling the Abiotic/Biotic Interface
- (19) Quantum Stochastics and Control
- (20) Qubit Enabled Imaging, Sensing & Metrology (QuISM)
- (21) Flex-Activated Materials
- (22) Game Theory for Adversarial Behavior
- (23) Light filamentation
- (24) Novel Free-Standing 2D Crystalline Materials (Oxides/Nitrides)
- (25) Value of Information for Distributed Data Fusion

Proposals from a team of university investigators may be warranted because the necessary expertise in addressing the multiple facets of the topics may reside in different universities, or in different departments in the same university. By supporting multidisciplinary teams, the program is complementary to other DoD basic research programs that support university research through single-investigator awards. Proposals shall name one Principal Investigator (PI) as the responsible technical point of contact. Similarly, one institution shall be the primary awardee for the purpose of award execution. The PI shall come from the primary institution. The relationship among participating institutions and their respective roles, as well as the apportionment of funds including sub-awards, if any, shall be described in both the proposal text and the budget.

### 7. Point(s) of Contact

One or more Research Topic Chiefs are identified for each specific MURI Topic. Questions of a technical nature shall be directed to one of the Research Topic Chiefs identified in Section VIII entitled, "Specific MURI Topics" of this BAA.

Questions of a *policy* nature for all three (3) services shall be directed to ONR as specified below:

ONR MURI Program Point of Contact: Dr. Bill Lukens MURI Program Manager Office of Naval Research, Code 03R E-mail Address: william.lukens1@navy.mil

Mailing address:
Office of Naval Research
One Liberty Center
875 North Randolph Street, Suite 1409
Arlington, VA 22203-1995

Questions of a *business nature* for all three (3) services shall be directed to the cognizant Contract Specialist, as specified below:

Primary:
Lynn Christian

Contract and Grants Awards Management, Code ONR 0251
Office of Naval Research
875 North Randolph Street, Suite W1273
Arlington, VA 22203-1995
E-Mail: lynn.christian@navy.mil

Secondary:
Vera M. Carroll
Acquisition Branch Head
Contract and Grants Awards Management, Code 0251
Office of Naval Research
875 North Randolph Street, Suite 1279
Arlington VA, 22203-1995
E-mail: vera.carroll@navy.mil

Questions submitted within 2 weeks prior to a deadline may not be answered, and the due date for submission of the white paper and/or full proposal will not be extended.

Answers to questions submitted in response to this BAA will be addressed in the form of an Amendment and will be posted to one or more of the following webpages:

- Grants.gov Webpage http://www.grants.gov/
- ONR Broad Agency Announcement (BAA) Webpage –
   <a href="http://www.onr.navy.mil/en/Contracts-Grants/Funding-Opportunities/Broad-Agency-Announcements.aspx">http://www.onr.navy.mil/en/Contracts-Grants/Funding-Opportunities/Broad-Agency-Announcements.aspx</a>

### 8. Instrument Type(s)

It is anticipated that all awards resulting from this announcement will be grants.

# 9. Catalog of Federal Domestic Assistance (CFDA) Numbers

12.300 ONR 12.800 AFOSR 12.431 ARO

### 10. Catalog of Federal Domestic Assistance (CFDA) Titles

Basic and Applied Scientific Research, (ONR)
Air Force Defense Research Sciences Program, (AFOSR)
Basic Scientific Research, (ARO)

#### 11. Other Information

The Non-ONR Agency Information:
Air Force Office of Scientific Research
875 North Randolph Street
Suite 325, Room 3112
Arlington, VA 22203-1768

Army Research Office 4300 S. Miami Blvd Durham. NC 27703-9142

# II. AWARD INFORMATION

It is anticipated the awards will be made in the form of grants to universities. The awards will be made at funding levels commensurate with the proposed research and in response to agency missions. Each individual award will be for a three year base period with one 2-year option period to bring the total maximum term of the award to five years. The base and option period will be incrementally funded.

Total amount of funding for five years available for grants resulting from this MURI BAA is estimated to be about \$230M, pending out-year appropriations. MURI awards are \$1M-\$1.5M per year, with the actual amount contingent on availability of funds, the specific topic, and the scope of the proposed work. With few exceptions an individual award may not exceed \$1.5M per year. It is strongly recommended that potential proposers communicate with the Program Topic Chief regarding these issues before the submission of formal proposals. Depending on the results of the proposal evaluation, there is no guarantee that any of the proposals submitted in response to a particular topic will be recommended for funding. On the other hand, more than one proposal may be recommended for funding for a particular topic.

For the past three years Congress has placed limits on the percentage of facilities and administrative (F&A) costs that can be paid by the government using basic research (6.1) funds. Currently F&A costs paid under contracts and grants for the performance of basic

research may not exceed 35 percent. It is not known at present whether a similar indirect cost restriction will apply to 6.1 funds in FY 2011 or thereafter.

# III. <u>ELIGIBILITY INFORMATION</u>

This MURI competition is open only to and full proposals are to be submitted only by, U.S. institutions of higher education (universities) including DoD institutions of higher education, with degree-granting programs in science and/or engineering.\* Ineligible organizations (e.g., industry, DoD laboratories, Federally Funded Research and Development Centers (FFRDCs), and foreign universities) may collaborate on the research but may not receive MURI funds, directly or via subaward.

When a modest amount of additional funding for an ineligible organization is necessary to make the proposed collaboration possible, such funds may be requested via a separate proposal from that organization. This supplemental proposal should be attached to the primary MURI proposal and will be evaluated separately by the responsible Research Topic Chief. If approved, the supplemental proposal will be funded by the responsible agency using non-MURI funds. Since it is not certain that non-MURI funding would be available for ineligible organizations, Principal Investigators are encouraged to restrict funding requests to eligible organizations when practical.

# IV. APPLICATION AND SUBMISSION INFORMATION

# 1. Application and Submission Process

The proposal submission process is in two stages. Prospective awardees are encouraged to submit white papers to minimize the labor and cost associated with the production of detailed full proposals that have very little chance of being selected for funding. Based on an assessment of the white papers, the responsible Research Topic Chief will provide informal feedback notification to the prospective awardees to encourage or discourage them to submit full proposals. The Topic Chief may also on occasion provide feedback encouraging reteaming to strengthen a proposal.

White papers arriving after the deadline may not receive feedback prior to full proposal submission. However, all full proposals submitted under the terms and conditions cited in the BAA will be reviewed.

<u>Due Date</u>: The due date for white papers is no later than 4:00 P.M. (Eastern Time) on Thursday, 30 September 2010.

#### Submission of White Papers:

White papers may be submitted via e-mail directly to a Research Topic Chief, via the United States Postal Service (USPS), via a commercial carrier or may be hand delivered to the attention of a responsible Research Topic Chief at the agency specified for the topic. For

<sup>\*</sup>To the extent that it is a part of a U.S. institution of higher education and is not designated as an FFRDC, a University Affiliated Research Center (UARC) or other University Affiliated Laboratory (UAL) is eligible to submit a proposal to this MURI competition and receive MURI funds. However, the eligibility of a UAL (other than an FFRDC) to submit a URI proposal does not exempt the proposal from any evaluation factor contained in this Broad Agency Announcement, to include the potential impact on the institution's ability to perform defense-relevant research and to train students in science and/or engineering.

hard copy submissions, use the addresses provided in Section IV entitled, "Application and Submission Information" paragraph number 6 entitled, "Address for the Submission of Hard Copy White Papers". White papers should be stapled in the upper left hand corner; plastic covers or binders should not be used. Separate attachments, such as individual brochures or reprints, will not be accepted.

<u>Evaluation/Notification</u>: Initial evaluations of the white papers will be issued on or about Tuesday, 12 October 2010.

### Submission of Full Proposal:

Any Offeror may submit a full proposal even if its white paper was not identified as being of "particular value" to the Government. However, the initial evaluation of the white papers should give prospective awardee some indication of whether a later full proposal would likely result in an award.

# NOTE: Full Proposals must be submitted electronically through grants.gov.

Registration Requirements for Grants.gov: There are several one-time actions you must complete in order to submit an application through Grants.gov (e.g., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the Central Contract Registry (CCR), register with the credential provider, and register with Grants.gov). See <a href="https://www.grants.gov/GetStarted">www.grants.gov/GetStarted</a> to begin this process. Use the Grants.gov Organization Registration Checklist at <a href="https://www.grants.gov/assets/OrganizationRegCheck.doc">www.grants.gov/assets/OrganizationRegCheck.doc</a> to guide you through the process. Designating an E-Business Point of Contact (EBiz POC) and obtaining a special password called an MPIN are important steps in the CCR registration process. Applicants, who are not registered with CCR and Grants.gov, should allow at <a href="least 21 days">least 21 days</a> completing these requirements. It is suggested that the process be started as soon as possible.

**Questions:** Questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@grants.gov.

### 2. Content and Format of White Papers and Full Proposals

The white papers and full proposals submitted under this BAA are expected to address unclassified basic research. White papers and full proposal submissions will be protected from unauthorized disclosure in accordance with applicable law and DoD regulations. Proposers are expected to appropriately mark each page of their submission that contains proprietary information. Grants awarded under this announcement shall be unclassified.

**Important Note:** Titles given to the White Papers/Full Proposals should be descriptive of the work they cover and not be merely a copy of the title.

### a. White Paper Submission: Contents and Format of Applications

Each topic in this announcement has one or more Research Topic Chiefs identified from one of the participating agencies; ONR, AFOSR, or ARO. You should submit your white paper to one of the Research Topic Chiefs at the agency for which you are applying.

White paper format should be as follows:

- Paper Size 8.5 x 11 inch paper
- Margins 1 inch
- Spacing single spaced
- Font Times New Roman, 12 point
- Number of Pages no more than four (4) single-sided pages (excluding cover letter, cover, and curriculum vitae). White papers exceeding the page limit may not be evaluated.

White Paper content should be as follows:

- A one page cover letter (optional)
- A cover page, labeled "PROPOSAL WHITE PAPER," that includes the BAA number, proposed title, and proposer's technical point of contact, with telephone number, facsimile number, e-mail address, topic number, and topic title
- · Identification of the research and issues
- Proposed technical approaches
- Potential impact on DoD capabilities
- Potential team and management plan
- Summary of estimated costs
- Curriculum vitae of key investigators

The white paper should provide sufficient information on the research being proposed (e.g., hypothesis, theories, concepts, approaches, data measurements and analysis, etc.) to allow for an assessment by a technical expert. It is not necessary for white papers to carry official institutional signatures.

Copies – one (1) original and two (2) copies.

### b. Grants.gov Full Proposal Submission: Content and Format of Applications

Application forms and instructions are available at Grants.gov. To access these materials, go to <a href="http://www.grants.gov">http://www.grants.gov</a>, select "Apply for Grants", and then select "Download Application Package". Enter the CFDA for the respective agency to which you are directing the application (ONR – 12.300, AFOSR – 12.800, ARO – 12.431), as found on page five of this announcement) and the funding opportunity number, designated as "research opportunity number" on page two of this announcement. Each topic in this announcement has a Research Topic Chief identified from one of the participating agencies; ONR, AFOSR, or ARO. You should direct your application to the agency associated with the topic for which you are applying.

# Content and Form of Application – SF 424 (R&R) - Mandatory

You must complete the mandatory forms in accordance with the instructions on the forms and the additional instructions below. Files that are attached to the forms must be in Adobe Portable Document Format (PDF) unless otherwise specified in this announcement.

# Form: SF 424 (R&R) - Mandatory

Complete this form first to populate data in other forms. Complete all the required fields in accordance with the pop-up instructions on the form. To activate the instructions, turn on the "Help Mode" (icon with the pointer and question mark at the top of the form). To be considered for award, applicants must fill out block 4 of the SF 424 R&R as follows: Block 4a "Federal Identifier": leave blank; Block 4b "Agency Routing Identifier": enter the appropriate topic chief's name.

### Form Research & Related Other Project Information - Mandatory

Complete questions 1 through 6 and attach files. The files must comply with the following instructions:

### **Project Summary/Abstract (Field 7 on the Form) - Mandatory**

The project summary should be a single page that identifies the research problem, technical approaches, anticipated outcome of the research, if successful, and impact on DoD capabilities. It should identify the Principal Investigator, the university and other universities involved in the MURI team if any, the proposal title, the agency to which the proposal is submitted, the MURI topic number and the total funds requested from DoD for the 3-year base period, the 2-year option period and the 5-year total period. The project summary must not exceed 1 page when printed using standard 8.5" by 11" paper with 1" margins (top, bottom, left and right) with font Times New Roman 12 point. To attach a Project Summary/Abstract, click "Add Attachment."

# Project Narrative (Field 8 on the form) - Mandatory

#### The Following Formatting Rules Apply for Field 8

- Paper size when printed 8.5 x 11 inch paper
- Margins 1 inch
- Spacing -single
- Font Times New Roman, 12 point
- Number of pages no more than twenty-five (25) single-sided pages.
   The cover, table of contents, list of references, letters of support, and curriculum vitae are excluded from the page limitations. Full proposals exceeding the page limit may not be evaluated.

### Include the Following in Field 8

The first page of your narrative must include the following information:

- Principal Investigator name
- Phone number, fax number and e-mail address
- Institution, Department, Division
- Institution address
- Other universities involved in the MURI team
- Current DoD Contractor or Grantee? If yes, provide Agency, point of contact; and phone number
- Proposal title

- Institution proposal number
- Agency to which proposal is submitted
- Topic number and topic title
- <u>Table of Contents</u>: List project narrative sections and corresponding page numbers.
- Technical Approach: Describe in detail the basic science and/or engineering research to be undertaken. State the objective and approach, including how data will be analyzed and interpreted. Discuss the relationship of the proposed research to the state-of-the-art knowledge in the field and to related efforts in programs elsewhere, and discuss potential scientific breakthroughs. Include appropriate literature citations/references. Discuss the nature of expected results. Discuss potential applications to defense missions and requirements. Describe plans for the research training of students. Include the number of full time equivalent graduate students and undergraduates, if any, to be supported each year. Discuss the involvement of other students, if any.
- <u>Project Schedule, Milestones and Deliverables</u>: A summary of the schedule of events, milestones, and a detailed description of the results and products to be delivered.
- <u>Management Approach</u>: A discussion of the overall approach to the management of this effort, including brief discussions of: required facilities; relationships with any subawardees and with other organizations; availability of personnel; and planning, scheduling and control procedures.
  - (a) Describe the facilities available for the accomplishment of the proposed research and related education objectives. Describe any capital equipment planned for acquisition under this program and its application to the proposed research. If possible, budget for capital equipment should be allocated to the first budget period of the grant. Include a description of any government furnished equipment/hardware/software/information, by version and/or configuration that are required for the proposed effort.
  - (b) Describe in detail proposed subawards to other eligible universities or relevant collaborations (planned or in place) with government organizations, industry, or other appropriate institutions. In particular, describe how collaborations are expected to facilitate the transition of research results to applications. Descriptions of industrial collaborations should explain how the proposed research will impact the company's research and/or product development activities. If subawards to other universities are proposed, make clear the division of research activities, to be supported by detailed budgets for the proposed subawards.
  - (c) Designate one individual as the Principal Investigator for the award, for the purpose of technical responsibility and to serve as the primary point-of-contact with an agency's Program Topic Chief. Briefly summarize the qualifications of the Principal Investigator and other key investigators to conduct the proposed research.
  - (d) List the amount of funding and describe the research activities of the Principal Investigator and co-investigators in on-going and pending research projects, whether or not acting as Principal Investigator in these other projects, the time charged

to each of these projects, and their relationship to the proposed effort.

- (e) Describe plans to manage the interactions among members of the proposed research team.
- (f) Identify other parties to whom the proposal has been, or will be sent, including agency contact information.
- List of References: List publications cited in above sections.
- <u>Letters of Support</u>: Up to three Letters of Support from various DoD agencies may be included.
- <u>Curriculum Vitae</u>: Include curriculum vitae of the Principal Investigator and key co-investigators.

**All applications should be in a single PDF file.** To attach a Project Narrative in Field 8, click "Add Attachment."

### Bibliography & References Cited (Field 9 on the form)

This field not required.

## Facilities & Other Resources (Field 10 on the form)

This field not required.

### Equipment (Field 11 on the form)

This field not required.

# Other Attachment (Field 12 on the form)

Attach budget proposal at field 12. You must provide a detailed cost breakdown of all costs, by cost category and by the funding periods described below, corresponding to the proposed Technical Approach which was provided in Field 8 of the Research and Related Other Project Information Form. The option must be separately priced. The Research and Related Budget form is not required.

The budget should adhere to the following guidelines:

Detailed breakdown of all costs, by cost category, by the calendar periods stated below. For budget purposes, use an award start date of 01 Junel 2011. For the three-year base grant, the cost should be broken down to reflect funding increment periods of:

- (1) Four months (01 Jun 11 to 30 Sep 11),
- (2) Twelve months (01 Oct 11 to 30 Sep 12),
- (3) Twelve months (01 Oct 12 to 30 Sep 13), and
- (4) Eight months (01 Oct 13 to 31 May 14).

Note that the budget for each of the calendar periods (e.g. 01 June 11 to 30 Sep 11) should include only those costs to be expended during that calendar period.

The budget should also include an option for two additional years broken down to the following funding periods:

- (1) Four months (01 Jun 14 to 30 Sep 14),
- (2) Twelve months (01 Oct 14 to 30 Sep 15), and
- (3) Eight months (01 Oct 15 to 31 May 16).

Annual budget should be driven by program requirements. Elements of the budget should include:

• <u>Direct Labor</u> – Individual labor categories or persons, with associated labor hours and unburdened direct labor rates. Provide escalation rates for out years.

Administrative and clerical labor – Salaries of administrative and clerical staff are normally indirect costs (and included in an indirect cost rate). Direct charging of these costs may be appropriate when a major project requires an extensive amount of administrative or clerical support significantly greater than normal and routine levels of support. Budgets proposing direct charging of administrative or clerical salaries must be supported with a budget justification which adequately describes the major project and the administrative and/or clerical work to be performed.

- Fringe Benefits and Indirect Costs (i.e., F&A, Overhead, G&A, etc) The proposal should show the rates and calculation of the costs for each rate category. If the rates have been approved/negotiated by a Government agency, provide a copy of the memorandum/agreement. If the rates have not been approved/negotiated, provide sufficient detail to enable a determination of allowability, allocability and reasonableness of the allocation bases and how the rates are calculated. Additional information may be requested, if needed. If composite rates are used, provide the calculations used in deriving the composite rates.
- <u>Travel</u> The proposed travel cost should include the following for each trip: the purpose of the trip, origin and destination if known, approximate duration, the number of travelers, and the estimated cost per trip must be justified based on the organizations historical average cost per trip or other reasonable basis for estimation. Such estimates and the resultant costs claimed must conform to the applicable Federal cost principals.
- <u>Subawards</u> Provide a description of the work to be performed by the subrecipients. For each subaward, a detailed cost proposal is required to be included in the principal investigator's cost proposal. Fee/profit is unallowable.
- <u>Consultants</u> Provide a breakdown of the consultant's hours, the hourly rate proposed, any other proposed consultant costs, a copy of the signed Consulting Agreement or other documentation supporting the proposed consultant rate/cost and a copy of the consultant's proposed statement of work if it is not already separately identified in the prime contractor's proposal.
- <u>Materials & Supplies</u> Provide an itemized list of all proposed materials and supplies including quantities, unit prices, proposed vendors (if known), and the basis for the estimate (e.g., quotes, prior purchases, catalog price lists).

- Recipient Acquired Equipment or Facilities Equipment and/or facilities are normally furnished by the Recipient. If acquisition of equipment and/or facilities is proposed, a justification for the purchase of the items must be provided. Provide an itemized list of all equipment and/or facilities costs and the basis for the estimate (e.g., quotes, prior purchases, catalog price lists). Allowable items normally would be limited to research equipment not already available for the project. General purpose equipment (i.e., equipment not used exclusively for research, scientific or other technical activities, such as personal computers, office equipment and furnishings, etc.) should not be requested unless they will be used primarily or exclusively for the project. For computer/laptop purchases and other general purpose equipment, if proposed, include a statement indicating how each item of equipment will be integrated into the program or used as an integral part of the research effort.
- Other Direct Costs Provide an itemized list of all other proposed other direct costs such as Graduate Assistant tuition, laboratory fees, report and publication costs and the basis for the estimate (e.g., quotes, prior purchases, catalog price lists).

<u>NOTE</u>: If the grant proposal is for a conference, workshop, or symposium, the proposal should include the following statement: "The funds provided by ONR will not be used for food or beverages."

• Fee/Profit – Fee/profit is unallowable.

### Funding Breakdown

Funding breakdown corresponding to the proposed Technical Approach which was provided in Field 8 of the Research and Related Other Project Information Form must also be attached.

### **Proposal Receipt Notices**

After a full proposal is submitted through Grants.gov, the Authorized Organization Representative (AOR) will receive a series of three e-mails. It is extremely important that the AOR <u>watch</u> for and <u>save</u> each of the e-mails. You will know that your proposal has reached ONR, ARO or AFOSR when the AOR receives e-mail Number 3. You will need the Submission Receipt Number (e-mail Number 1) to track a submission. The three e-mails are:

Number 1 – The applicant will receive a confirmation page upon completing the submission to Grants.gov.

Number 2 – The applicant will receive an e-mail indicating that the proposal has been validated by Grants.gov within two days of submission. (This means that all of the required fields have been completed.)

Number 3 – The third notice is an acknowledgment of receipt in e-mail form from the designated agency within ten days from the proposal due date. The e-mail is sent to the authorized representative for the institution. The e-mail for proposals notes that the proposal has been received and provides the assigned tracking number.

# 3. Significant Dates and Times

Schedule of Events		
Event	Date	Time
Questions Regarding white papers	16 September 2010*	2:00PM Eastern Time
White Papers Due	30 September 2010	4:00 PM Eastern Time
Notification of Initial DoD Evaluations of White Papers	12 October 2010**	
Questions Regarding full proposals	23 November 2010*	2:00PM Eastern Time
Full Proposals Due	07 December 2010	4:00 PM Eastern Time
Notification of Selection for Award	18 March 2011**	
Start Date of Grant	01 June 2010*	

<sup>\*</sup>Questions received after this date and time may not be answered, and the due date for submission of the proposals will not be extended

**Note:** Due to changes in security procedures since September 11, 2001, the time required for hard-copy written materials to be received at the Office of Naval Research has increased. Materials submitted through the U.S. Postal Service, for example, may take seven days or more to be received, even when sent by Express Mail. Thus, any hard-copy proposal should be submitted long enough before the deadline established in the solicitation so that it will not be received late and thus be ineligible for award consideration.

# 4. Submission of Late Proposals

Any full proposal submitted and validated through Grants.gov where the time and date for submission (e-mail Number #2) is after the deadline for proposal submission in Section IV entitled, "Application and Submission Information" paragraph number 3 entitled, "Significant Dates and Times" will be late and will not be evaluated unless the Grants.gov website was not operational on the due date and was unable to receive the proposal submission. If this occurs, the time specified for the receipt of proposals through Grants.gov will be extended to the same time of the day specified in this BAA on the first workday on which the Grants.gov website is operational.

Be advised that Grants.gov applicants have been experiencing system slowness and validation issues which may impact the time required submitting proposals. After proposals are uploaded to grants.gov, the submitter receives an email indicating the proposal has been submitted and that grants.gov will take up to two days to validate the proposal. As it is possible for grants.gov to reject the proposal during this process,

<sup>\*\*</sup> These dates are estimates as of the date of this announcement.

it is STRONGLY recommended that any soft-copy proposals be uploaded at least two days before the deadline established in the solicitation so that it will not be received late and be ineligible for award consideration.

a. For ARO, use the following alternative to submitting proposals to grants.gov.

Email your completed proposal package and grants.gov trouble ticket/case number to aror.baa@us.army.mil Your proposal must include all signatures and attachments and be submitted in PDF format. All proposal submissions will be subsequently evaluated by ARO for completeness and an official email confirmation will be sent. Incomplete packages will not be considered for an award. All submissions must meet the deadline specified in the BAA

- b. For AFOSR submissions please email your completed proposal package and grants.gov trouble ticket/case number to proposal@afosr.af.mil. Each email may not exceed 35MB. If necessary, use multiple emails sending the full proposal noting the trouble ticket/case number. Your proposal must include all signatures and attachments and be submitted in PDF format. An auto-reply email will be returned to the sender indicating that your email arrived. All proposal submissions will be subsequently evaluated by AFOSR for completeness and an official email confirmation will be sent. Incomplete packages will not be considered for an award. All submissions must meet the deadline of 4:00 (Eastern Time) 02 March 2010.
- c. There is no alternative process for ONR. Full proposals must be submitted through grants.gov

# 5. Address for Submission of Hard Copy White Papers

Submission of white papers shall be sent to the addresses below:

## **Important Notes Regarding Submission of Hard Copy White Papers:**

If the Offeror is using USPS, please allow an additional five (5) business days for the package to be delivered due to USPS mail being sent to a central location for special processing before it is sent to the addresses below.

### Office of Naval Research:

Hard copies of white papers topics (1) to (10) should be sent to the Office of Naval Research at the following address: For those topics with multiple topic chiefs, send the white paper to the first topic chief listed.

Primary:

Office of Naval Research
ATTN: (list name of responsible Research Topic Chief)
875 North Randolph Street - Suite W256A\*
Arlington, VA 22203-1995
Point of Contact: Paula Barden
Email: paula.barden.ctr@navy.mil
703-696-4111

#### Secondary:

Office of Naval Research
ATTN: (list name of responsible Research Topic Chief)
875 North Randolph Street - Suite 1409\*
Arlington, VA 22203-1995
Point of Contact: Dr. William Lukens
Email: William.lukens1@navy.mil
703-696-4668

\*This is the address for hand delivery, delivery via USPS and delivery via commercial delivery services.

If a telephone number is required, please use 703-696-4111 or 703-696-4668.

#### Air Force Office of Scientific Research:

Hard copy white papers addressing topics (11) to (17) should be sent to the Air Force Office of Scientific Research at the following address:

Air Force Office of Scientific Research
ATTN: (list name of responsible Research Topic Chief)
875 North Randolph Street
Suite 325, Room 3112
Arlington, VA 22203-1768
Point of Contact: Dr. Spencer Wu
703-696-7315
Email: spencer.wu@afosr.af.mil

#### U.S. Army Research Office:

Hard copy white papers addressing topics (18) to (25) should be sent to the U.S. Army Research Office at one of the following addresses:

For delivery by USPS (ordinary First Class or Priority Mail (but not Express Mail)):

U.S. Army Research Office (FY11 MURI)
P. O. Box 12211
Research Triangle Park, NC 27709-2211
Email: larry.russelljr@us.army.mil

For commercial delivery (such as Express Mail, FedEx, UPS, etc.):

U.S. Army Research Office (FY11 MURI)
For white papers include: ATTN: (list name of responsible Research Topic Chief)
4300 S. Miami Blvd
Durham, NC 27703-9142
919-549-4211
Email: larry.russelljr@us.army.mil

NOTE: White Papers sent by fax will not be considered.

#### V. EVALUATION INFORMATION

### 1. Evaluation Criteria

A. Basic Research: The MURI Program is funded by basic research (Budget Activity 1) money. White papers and full proposals, **in order to be considered for funding**, are therefore required to be of a basic, rather than applied or advanced technological, nature. Note that basic research includes "scientific study and experimentation directed toward increasing fundamental knowledge and understanding" while applied research deals with "the development of useful materials, devices, and systems or methods" and "the design, development, and improvement of prototypes and new processes to meet general mission requirements." The full definitions of these terms are contained in the links http://comptroller.defense.gov/fmr/02b/02b\_05.pdf

White papers will be evaluated by the responsible Research Topic Chief to assess whether the proposed research is likely to meet the objectives of the specific topic, and thus whether to encourage the submission of a full proposal. The assessment will focus on scientific and technical merit (criterion 2, below) and potential DoD interest and contribution to the topical area of science (criterion 3, below), although the other criteria may also be used in making the assessment.

Full proposals responding to this BAA in each topic area will be evaluated using the following criteria. The first four evaluation factors are of equal importance:

- (1) the qualifications and availability of the Principal Investigator and key coinvestigators;
- (2) scientific and technical merits of the proposed basic science and/or engineering research;
- (3) potential DoD interest and contribution to the topical area of science; and
- (4) potential impact on the institution's ability to perform defense-relevant research and to train, through the proposed research, students in science and/or engineering (for example, by acquiring or refurbishing equipment that can support DoD research and research-related educational objectives).

The following three evaluation criteria are each of lesser importance than any of the above four, but are equal to each other:

- (5) the adequacy of current or planned facilities and equipment to accomplish the research objectives;
- (6) the impact of interactions with other organizations engaged in related research and development, in particular DoD laboratories, industry, and other organizations that perform research and development for defense applications; and
- (7) the realism and reasonableness of cost (cost sharing is not a factor in the evaluation).

Decisions for exercising options will be based on accomplishments during the base years and potential research advances during the option years that can impact DoD research priorities and technological capabilities.

### 2. Evaluation Panel

White papers will be reviewed either solely by the responsible Research Topic Chief for the specific topic or by an evaluation panel chaired by the responsible Research Topic Chief. An evaluation panel will consist of technical experts who are Government employees or who are specialized government employees secured under the Intergovernmental Personnel Act (IPA). These individuals will sign a conflict of interest statement prior to receiving proposal information.

Full proposals will undergo a multi-stage evaluation procedure. The cognizant Program Officer and other Government scientific experts will perform the evaluation of technical proposals first. Cost proposals will be evaluated by Government business professionals. Restrictive notices notwithstanding, one or more support contractors or peers from the university community may be utilized as subject-matter-expert technical consultants. Similarly, support contractors may be utilized to evaluate cost proposals. However, proposal selection and award decisions are solely the responsibility of Government personnel. Each support contractor's employee and peer from the university community having access to technical and cost proposals submitted in response to this BAA will be required to sign a non-disclosure statement prior to receipt of any proposal submission. Findings of the evaluation panels will be forwarded to senior DoD officials who will make funding recommendations to the awarding officials.

Due to the nature of the MURI program, the evaluation panels and reviewing officials may on occasion recommend that less than an entire MURI proposal be selected for funding. This may be due to several causes such as insufficient funds, research overlap among proposals received, or potential synergies among proposals under a research topic. In such cases, proposal adjustments will be agreed by the Principal Investigator and the government prior to final award.

### **VI. AWARD ADMINISTRATION INFORMATION**

### 1. Administrative Requirements –

- CCR Successful Offerors not already registered in the Central Contractor Registry (CCR) will be required to register in CCR prior to award of any grant. Information on CCR registration is available at <a href="https://www.bpn.gov/ccr/default.aspx">https://www.bpn.gov/ccr/default.aspx</a>
- Certifications Grant awards greater than \$100,000 require a certification of compliance
  with a national policy mandate concerning lobbying. Grant applications shall provide this
  certification by electronic submission of SF424(R&R) as a part of the electronic proposal
  submitted via Grants.gov (complete Block 17). The following certification applies to each
  applicant seeking federal assistance funds exceeding \$100,000:

### **CERTIFICATION REGARDING LOBBYING ACTIVITIES**

- (1) No Federal appropriated funds have been paid or will be paid by or on behalf of the applicant, to any person for influencing or attempting to influence an officer or employee of an agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any Federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.
- (2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the Federal contract, grant, loan, or cooperative agreement, the applicant shall complete and submit Standard Form-LLL, "Disclosure Form to Report Lobbying," in accordance with its instructions.
- (3) The applicant shall require that the language of this certification be included in the award documents for all subawards at all tiers (including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements) and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by Section 1352, title 31, U.S.C. Any person who fails to file the required certification shall be subject to a civil penalty of not less than \$10,000 and not more than \$100,000 for each such failure.

#### Grants not through Grants.gov

Proposers seeking grants who have received Grants.gov waiver approval for awards greater than \$100,000 shall complete and submit electronic representations and certifications at the Contracts and Grants Section of the ONR Home Page at <a href="http://www.onr.navy.mil/Contracts-Grants/submit-proposal/~/media/BDBA1ACF9F534C10BE2A9C9AD9AA7F12.ashx">http://www.onr.navy.mil/Contracts-Grants/submit-proposal/~/media/BDBA1ACF9F534C10BE2A9C9AD9AA7F12.ashx</a>.

### 2. Reporting

In general, for each grant award, annual reports and a final report are required summarizing the technical progress and accomplishments during the performance period, as well as any other report as requested by the Research Topic Chief.

#### VII. OTHER INFORMATION

# 1. Government Property/Government Furnished Equipment (GFE) and Facilities

Government research facilities and operational military units are available and should be considered as potential government-furnished equipment/facilities. These facilities and resources are of high value and some are in constant demand by multiple programs. It is unlikely that all facilities would be used for any one specific program. The use of these facilities and resources will be negotiated as the program unfolds. Offerors should explain as part of their proposals which of these facilities are critical for the project's success.

# 2. Use of Animals and Human Subjects in Research

If animals are to be utilized in the research effort proposed, the Offeror must complete a DoD Animal Use Protocol with supporting documentation (copies of AAALAC accreditation and/or NIH assurance, IACUC approval, research literature database searches, and the two most recent USDA inspection reports) prior to award. For assistance with submission of animal research related documents, contact the ONR Animal Use Administrator at (703) 696-4046.

Similarly, for any proposal for research involving human subjects, the Offeror must submit or indicate an intention to submit prior to award: documentation of approval from an Institutional Review Board (IRB); IRB-approved research protocol; IRB-approved informed consent form; proof of completed human research training (e.g., training certificate or institutional verification of training); an application for a DoD-Navy Addendum to the Offeror's DHHS-issued Federal wide Assurance (FWA) or the Offeror's DoD-Navy Addendum. In the event that an exemption criterion under 32 CFR.219.101 (b) is claimed, provide documentation of the determination by the Institutional Review Board (IRB) Chair, IRB vice Chair, designated IRB administrator or official of the human research protection program including the category of exemption and short rationale statement. This documentation must be submitted to the ONR Human Research Protection Official (HRPO), by way of the ONR Program Officer. Information about assurance applications and forms can be obtained by contacting ONR 343 contact@navy.mil. If the research is determined by the IRB to be greater than minimal risk, the Offeror also must provide the name and contact information for the independent medical monitor. For assistance with submission of human subject research related documentation, contact the ONR Human Research Protection Official at (703) 696-4046.

For contracts and orders, the award and execution of the contract, order, or modification to an existing contract or order serves as notification from the Contracting Officer to the Contractor that the HRPO has approved the assurance as appropriate for the research under the Statement of Work and also that the HRPO has reviewed the protocol and accepted the IRB approval or exemption determination for compliance with the DoD Component policies. See, DFARS 252.235-7004.

#### 3. Recombinant DNA

Proposals which call for experiments using recombinant DNA must include documentation of compliance with Department of Human and Health Services (DHHS) recombinant DNA regulations, approval of the Institutional Biosafety Committee (IBC), and copies of the DHHS Approval of the IBC letter.

### 4. Department of Defense High Performance Computing Program

The DoD High Performance Computing Program (HPCMP) furnishes the DoD S & T and DT & E communities with use-access to very powerful high performance computing systems. Awardees of ONR contracts, grants, and assistance instruments may be eligible to use HPCMP assets in support of their funded activities if ONR Program Officer approval is obtained and if security/screening requirements are favorably completed. Additional information and an application may be found at <a href="http://www.hpcmo.hpc.mil/">http://www.hpcmo.hpc.mil/</a>.

# 5. Project Meetings and Reviews

Individual program reviews between the ONR sponsor and the performer may be held as necessary. Program status reviews may also be held to provide a forum for reviews of the latest results from experiments and any other incremental progress towards the major demonstrations. These meetings will be held at various sites throughout the country. For costing purposes, offerors should assume that 40% of these meetings will be at or near ONR, Arlington, VA and 60% at other contractor or government facilities. Interim meetings are likely, but these will be accomplished via video telephone conferences, telephone conferences, or via web-based collaboration tools.

# 6. Other Guidance, Instructions and Information

None

# VIII. SPECIFIC MURI TOPICS

#### ONR FY2011 MURI TOPIC # 1

Submit white papers and proposals to the Office of Naval Research

# **Soil Blast Modeling and Simulation**

Background: The accurate modeling and simulation of the output of buried explosive devices has yet to be adequately solved, and this information is vital to codes that use these results to analyze and design future vehicle requirements and vehicle designs. Eulerian incompressible and compressible hydrocodes have been developed to model explosive blasts in soil with good agreement to experimental data for dry or saturated sand using a frictional-cohesive viscoplastic model. Arbitrary Euler-Lagrange (ALE) numerical solvers have also been successfully developed to model explosive blast outputs in saturated sand with less than 7% experimental error. Despite limited successes, these methods are far from being universally accepted predictive tools, reliable enough to forgo experimental tests. One difficulty with modeling of more complex soils is its dual nature to behave as a solid or as a fluid under different loading conditions. Most existing models either treat the soil as an elastic-plastic solid, or as a non-Newtonian fluid, but are unable to treat the transition between the phases. A second difficulty arises with the time scale required to correctly predict the loading from a buried charge. While the initial shock and soil impact usually occurs on the order of a millisecond or less (depending on scale) the full loading due to soil cavity expansion interacting with the structure occurs over a period 10 to 100 times longer (depending on burial depth).

The loading function of an underground blast and resulting soil ejecta on structural surfaces above the ground has also been demonstrated to be nonlinear and is likely highly dependent on the soil type. The full development of a high fidelity multimaterial, multiphysics numerical solution to blasts in varying heterogeneous soil types, soil hydration levels, and depth of burial is a much more complex problem that has yet to be sufficiently solved. New focused research efforts are required to solve challenging computational continuum dynamics problems accurately while demonstrating a strong degree of computational efficiency. Of interest to this MURI are the development, implementation, and experimental validation of accurate soil material models in efficient, high fidelity explicit dynamic solvers. The new soil models should include equations of state, strength, and failure models developed for several representative soil types at the high strain rates observed during blast events. The performance of soil models during blast events must provide accurate results as a function of the depth of burial and properly characterize the resulting crater depth and diameter. Accuracy of the model should also be measured in terms of conservation of energy and momentum of the numerical solver's results. Additionally, the model will be validated using small-scale and full-scale blast events as well as literature data.

**Objective:** The objective of this MURI is to develop and validate a computationally efficient multimaterial, multiphysics explicit dynamics model that accurately represents explosive blasts of varying charge sizes and at various depths of burial in a diverse set of representative set of real-world heterogeneous soil types. This model will capture the dynamic transitions between elastic-plastic solid and non-Newtonian fluid behavior in a time scale required to correctly predict the loading from a buried charge. The results of this solver will serve as the boundary conditions for additional fluid structural interactions of the blast effects with deformable vehicle surfaces (ongoing MURI and vast background of previous work).

Research Concentration Areas: Selected research areas include, but are not limited to: (i) experimental characterization of a representative set of soils to capture nonlinear material properties as a function of pressure, strain rate, and internal energy; (ii) theoretical development and validation of new heterogeneous soil material models at high strain rates; (iii) incorporation of new soil material models into coupled Euler-Lagrange or mesh-free numerical explicit dynamics solvers; (iv) studying the performance of soil models in blast events as a function of depth; (v) studying and modeling the effects of fragmentation propagating through the soil overburden; (vii) the incorporation of results from particulate mechanics models into continuum models; and (vi) experimental testing to validate accuracy of explicit dynamics solutions.

**Impact:** Landmines and Improvised Explosive Devices are a major threat to the survivability of light vehicles and present a significant challenge to designing and building survivable platforms because of the large loads applied to the targets. Future vehicle designs can be significantly improved through the rapid iteration of computationally efficient blast simulations to accurately predict the output of buried charges and the response of target of interest.

Research Topic Chiefs: Mr. Lee Mastroianni, ONR, (703) 696-3073, <a href="mastroianni@navy.mil">lee.mastroianni@navy.mil</a>, Dr. David Shifler, ONR, (703) 696-0285, <a href="mastroianni@navy.mil">david.shifler@navy.mil</a>, and Maj. Billy Short, ONR, (703) 696-0155, <a href="mastroianni@navy.mil">billy.short@navy.mil</a>.

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# **Knowledge Representation and Reasoning for Decentralized Autonomy**

Background: Surveillance of unconstrained environments with decentralized teams of networked autonomous (sensing and information gathering) agents is a challenging problem that has a wide variety of applications. The purpose is to detect mission-relevant classes of entities and behaviors. and infer their activities, relationships and intentions. While much progress is being made in the study of network communication and control, computational theory needed for semantic understanding of the situation using teams of autonomous sensing and information gathering agents is at its infancy. It requires decentralized methods for optimal and continual replanning and reallocation of scarce resources to collect and process relevant information, and for aligning and aggregating individual agent perceptions, which are local and partial, to form a comprehensive consensus-based global understanding of the situation. Moreover, those methods must address hard challenges such as, gaps in data and various sources and types of uncertainty including data that is imprecise, incomplete, incorrect, contradictory, as well as communications latency and possibly deception. Also, networks of agents tend to gather massive amounts of data, much of which is irrelevant. Reasoning and learning obviously play key roles in dealing with these difficulties for arriving at correct understanding of the situation. Other major aspects of surveillance, namely, how individual agents perceive their local environments and how the system interacts with users are not the primary focus of this topic.

<u>Objective:</u> The objective is to develop theoretically well-founded and computationally efficient approaches for building decentralized teams of autonomous agents operating in dynamic, uncertain, unconstrained environments over extended time periods with minimal human supervision. In particular, we want to develop principled, robust methods with provable performance guarantees for the design of an overall system architecture that is scalable, allows dynamic formation of loosely coupled teams of agents, and enables optimal management of information in decentralized environments, as well as methods for knowledge and uncertainty representation, and decentralized reasoning and learning.

Research Concentration Areas: We envision multi-disciplinary basic research that draws from mathematics, artificial intelligence, control theory, computer and information sciences. Research areas include the following. (a) Methods for representation of mission intent and context that is understandable at mission level and actionable at the agent level. (b) Methods for representation of environmental context that describes expected entities, behaviors, relationships, and activities. (c) Methods for building knowledge bases from multiple uncertain sources that allow life-long learning, knowledge update and belief revision, and are optimized for inference. (d) Hierarchical architectures for decentralized team formation and control that address scalability and information sharing and management in decentralized teams. (e) Methods for robust decentralized reasoning and planning under information uncertainty. (e) Methods for meta-reasoning and introspection to assess own performance and seek help when needed, or determine if a task is impossible to achieve.

<u>Impact:</u> This research topic will advance the science necessary for developing and deploying lightly supervised versatile teams of autonomous agents for robust persistent, pervasive surveillance of unconstrained environments, such as the maritime domain, urban areas, riverine areas, littorals, etc.

Research Topic Chiefs: Dr. Behzad Kamgar-Parsi, ONR 311, 703-696-5754,

<u>behzad.kamgarparsi@navy.mil</u>; Dr. Jason Stack, ONR 321, 703-696-2485, <u>jason.stack@navy.mil</u>; Mr. Marc Steinberg, ONR 351, 703-696-5115, <u>marc.steinberg@navy.mil</u>.

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# III-Nitride Terahertz Electronics--Scaling strategies beyond Silicon

Background: Gallium Nitride (GaN) and related Group III-Nitrides have demonstrated remarkable advances in RF performance over the past decade, both in power output and frequency response. Currently, this materials system is the leading contender for uppermillimeter wave applications (DARPA is initiating the NEXT program to push these materials to the 500GHZ regime), exceeding all other III-V and group IV materials by nearly an order of magnitude in operating voltage, which largely results from the much higher critical breakdown field. Due to the limits of conventional device geometries, electron, transport studies in these high fields are challenging and will require fundamental research to extend the experimental methodology and the models used to extract the basic parameters. Looking at conventional scaling strategies to extend the application of these materials to the Terahertz region for high speed devices, the frequency ranges accessible to GaN-based electronics approach wavelength regimes that are beyond our current conceptualization of electronic semiconductor devices. The goal of this MURI topic is to enable the exploration of new electronic approaches for group III-Nitride structures capable of manipulating terahertz electromagnetic signals using principles that derive from electronic concepts. (Fundamentally, utilize energy provided in a low frequency form to control or amplify higher frequency energy)

**Objective:** Investigate device structures that exploit the high breakdown fields of III-Nitrides where electron transport properties are not limited (as current device geometries are) by scaling limitations as the operating frequencies are pushed up into the terahertz range while maintaining operating voltage. It is clear that Nitrides could have a significant impact at very high frequencies; the question is how to get there. If GaN-based devices are scaled like silicon and GaAs, the inherent limitations of those scaling approaches may result in a technology which is no better.

Research Concentration Areas: The opportunity presented here is to take a fresh look at electronics, unconstrained by the current known state of the art. As such, a broad set of disciplines can be expected to contribute and collaborate in this effort. Solid state devices themselves will require the expertise of material scientists, experimental and theoretical device physicists and engineers, along with knowledge in the current limitations of the state of the art. Novel approaches that exploit sub band levels of reduced-dimensional structures should be considered. In addition, these devices can be expected to be intimately tied to the electromagnetic (EM) environment both within and outside the solid state environment, thus the physics and engineering disciplines that specialize in EM theory will likely contribute. All of the known issues such as power dissipation, efficiency need to be considered, but the primary goal should be the search for concepts that are able to provide voltage and power gain, and significant output powers at > 1 Terahertz.

**Impact:** Power generation/amplification in the terahertz region lies at the upper limit of electronics, and lower limit of solid state optical approaches. Success in this MURI would lay out a path to an electronics solution for terahertz sensor applications. Secondly, an electronics platform would be available for the development of very high speed, high noise margin, signal processing.

### **Research Topic Chiefs:**

Dr. Paul Maki, ONR, 703-696-3060, paul.maki@navy.mil Dr. Dan Green, ONR, 703-696-4220, daniel.s.green1@navy.mil

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# **Charge Transport in DNA Molecular Wire**

Background: Potential of DNA (DeoxyriboNucleic Acid) as a functional material, beyond being the very molecule that codes Life itself, has been recognized for several decades. In recent years, particularly the last 3-5 years, progress has accelerated toward building various nanostructures using DNA. Today, arbitrary shaped two-dimensional (2D) structures with ~1nm fidelity, as well as various sophisticated 3D constructs, can be built with relative ease by folding long single strand DNA utilizing the famous Watson-Crick base pairing mechanism. At the same time, these DNA nanostructures perform very little in terms of functionality, particularly electronic functionality. Part of the reason is that, despite many years of study, a systematic electronic characterization of DNA molecule is still lacking. Existing data on charge transport through a DNA chain varies widely and remain controversial -- reports ranging from insulating, semiconducting to metallic and even superconducting behavior are common in the literature. Added to the confusion, and partially responsible for it, is the extreme sensitivity of DNA electrical transport properties to its external environment and other details of the experimental conditions. Recent advances in experimental techniques, such as availability of reliable contacts, as well as the exquisite control over its structures as mentioned above, makes a careful electronic characterization of DNA molecule both feasible and timely.

**Objective:** This MURI seeks a thorough and systematic electrical characterization of DNA molecule, with the aim to clarify and understand the fundamental mechanism for charge transport in DNA under various experimental conditions. The long-term goal, if sufficient understanding and control of electronic transport in DNA can be established, is to utilize these characterization data to design and construct various 2D and 3D DNA nanostructures with unique electronic functionalities.

Research Concentration Areas: Areas of interest include, but are not limited to: (1) Systematic electrical transport measurement in natural DNA by identifying and varying all relevant experimental parameters, both internal (base sequence, length, structure etc.) and external (contacts, medium, substrates etc.) to the DNA molecule. (2). A tightly integrated theoretical and modeling effort that aims to help understand experimental observations and also goes beyond to develop predictive theory and models to guide further experimentation. (3). In addition to the naturally occurring 4-letter DNA alphabet (Adenine, Thymine, Cytosine and Guanine), other DNA derivatives such as base modification or synthetic DNA bases are allowable, provided that they bring clear advantage in terms of superior electronic properties and compatible with the current structural DNA nanotechnology paradigm. (4). While electrical characterization of existing DNA nanostructures can be considered, this MURI will NOT entertain design and building of new structures unless the new structure has native electronic functionality built into it. (5). This MURI is about electrical characterization of DNA molecule itself (natural or its derivatives). Using various DNA nanostructures as scaffolds to assemble other electronic materials (therefore add electronic functionality) is an important research topic being addressed elsewhere, and therefore will NOT be considered in this MURI.

**Impact:** DNA nanostructures are among the smallest nanosystems men can build today with predictability, reasonable throughput, yield and cost. If the MURI succeeds in establishing useful level of electrical conductivity through DNA molecules, one can combine it with the recent advances in structural DNA nanotechnology to build highly functional nanosystems that

undoubtedly will lead to revolutionary new capabilities for future warfighters.

Research Topic Chiefs: Dr. Chagaan Baatar, ONR 312, (703)-696-0483. <a href="mailto:chagaan.baatar@navy.mil">chagaan.baatar@navy.mil</a>.

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# **Coupled Human-Landscape Interactions in Low-lying Coastal Environments**

**Background:** Humans occupying marginal terrain in many economically challenged countries are highly vulnerable to fluctuations in the natural environment. Both natural disasters and such slower natural changes as sea level rise may drastically increase the susceptibility of low-lying coastal populations to political instability. Understanding and predicting the mobility of such disadvantaged populations in response to a changing landscape is made increasingly possible by a number of new developments: patterns of human mobility in developed countries are amenable to study through tracking of cell phone activity; dissemination of information by phone, email and other networks, both physical and electronic, has been studied extensively using epidemiological concepts; ready availability of high resolution remote sensing imagery; and multi-agent system models of land-use change which have been applied to urban sprawl and development. The physical properties of a changing landscape, in particular, changes in the availability of habitable land and transportation routes to reach habitable land (which may be over water), are very strongly coupled to human mobility.

**Objective:** Develop a predictive model for the coupled interaction of the evolving physical landscape and the socio-econo-politically driven migratory response of populations affected by rising sea level in low-lying coastal areas. Determine the level of physical model fidelity required to adequately describe landscape evolution over relevant time and space scales. Likewise, determine the level of socio-econo-political modeling needed to address human migration issues. Identify and model sources of information that drive human/population mobility and identify possible thresholds (which may be physical, cultural or political) that initiate migration. Incorporate the dominant conditions or influences that stimulate shifts in decision frameworks over time at the individual. group/network and society levels. Use the resulting model to predict or explain how information availability and social thresholds differ for catastrophic events (e.g., tsunami) versus slower processes (e.g. rising water table); how sources and mechanisms of information transfer in populations change during displacement and afterwards. Model development should be accompanied by ancillary studies of data sources for model input and validation, including capability for both quantitative and qualitative data constructs. Finally, consider how disparate data sources (e.g. cell phone activity, remote sensing imagery and social network applications, among others) might be assimilated into predictive models to anticipate social / political / economic disruption and predict migration patterns.

Research Concentration Areas: This MURI requires multidisciplinary collaborative investigations that will require environmental prediction and remote sensing expertise in coastal, nearshore, riverine and deltaic systems; expertise in social networks and epidemiology; expertise in multi-agent and systems dynamic models, to generate predictive models for human population mobility in response to changing natural landscapes. Data-assimilative models of dynamic social, economic, and political that are fundamentally coupled to spatial and temporal descriptions of the physical environment are required for fundamental progress.

**Impact:** New understanding of individual, group and population responses to natural changes in the landscape will provide the potential to predict future response to a rising sea level that will affect hundreds of millions of disadvantaged people in low-lying areas and countries already susceptible to political instability. New knowledge will improve DoD and civilian response to natural and manmade disasters, an increasingly prominent aspect of humanitarian aid.

**Research Topic Chiefs:** Dr. Tom Drake, ONR 322, 703-696-1206, tom.drake@navy.mil and Dr. Ivy Estabrooke, ONR 30, 703-588-2396, ivy.estabrooke@navy.mil

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# **Integrated Oceanographic, Atmospheric, and Acoustic Physics**

### **Background**

To date the challenges of understanding the physics of meteorology, oceanography and acoustics have been separately addressed with results for one field being used sequentially in the other fields of study. However, the starting point for each field of study is the same, i.e., the Navier-Stokes equations. Specializations of those equations (e.g., assuming incompressibility of the fluid, treating only the hydrostatic pressure, ignoring gravity) have made it possible to make progress at the cost of separating fields of study. Physical understanding has advanced to the point that integrated basic science efforts can now be envisioned. As an example, recent inclusion of non-linear, non-hydrostatic terms in the oceanography of continental slopes have allowed a better understanding of non-linear internal wave generation and propagation in real world environments. Adding fluid compressibility to this type of research will allow a synoptic understanding of acoustic propagation within this environment.

# **Objective**

The initiative will develop the integrated physics required to include boundaries, initial conditions and forcing functions and synoptically examine time evolution of 3D linear and non-linear physics in both the fluid flow and acoustic propagation in the ocean and the atmosphere.

#### **Research Concentration Areas**

The research of this initiative will concentrate on: 1) incorporating fluid compressibility (the physics of acoustics) into the Navier-Stokes equations used in analyses of sub-mesoscale processes (i.e., linear and non-linear internal waves) within realistic 3D oceanographic and/or atmospheric environments, 2) understanding spatial and temporal evolution of both the physical state and of the acoustics transmitted within these heterogeneous, evolving environments, 3) testing this new understanding using data sets of opportunity, e.g., the shallow water acoustics experiment in 2006.

# **Impact**

Physical oceanography and meteorology have their independent utility to Navy operations and a large amount of effort has been put into ocean and weather forecasts. However, sonar operations occur within this same complex and ever changing ocean/atmosphere environment. The ability to understand and forecast within a single physical picture will allow new assessments of Navy system (e.g., ASW, MCM) performance metrics and the evolution of those metrics with time and space. These assessments will not need to begin with a priori judgments of relevant physics to include. This same physical picture will be useful in examining inversion schemes designed to determine parameters (directly from Navy sonars) to be used in more operationally oriented tactical decision aids.

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# **Improved Meterological Modeling in Mountainous Terrain**

**Background**: Complex topography profoundly affects local weather, yet remains an understudied problem. While advancements have been made in weather prediction on large spatial scales, knowledge gaps continue to challenge the fidelity of local predictions in the areas of complex terrain. Prediction of flow, turbulence, dispersion and extreme conditions is difficult because of many processes covering a broad spectrum of space-time scales. The applicability of conventional sub-grid parameterizations is in question while the role of sub-grid processes is more crucial than elsewhere. A lack of observations hampers prediction but necessitates forecasts that are more reliant on models. Four main topics (listed below) require increased fundamental research in order to improve modeling and predictions.

**Objective:** The objective of this MURI is to gain improved understanding of the dynamics of weather in mountainous terrain and to improve the realistic representation of the important processes in NWP models in order to improve their predictive skill.

#### **Research Concentration Areas:**

- 1. Model Core Issues: Space-time resolution is critical and unresolved scales lead to numerous problems. Methods using variable resolution, optimal coordinate systems and nesting need to be studied. One-way nesting (down scaling) is common, but the preponderance of energy production in small scales may lead to upscale transfer of properties, requiring two-way nesting.

  2. Boundary Conditions: Improved information on land use/cover and surface properties are needed. Shadowing creates space-time heterogeneities, which impact fluxes and radiation. The vertical variability of the surface creates serious issues, and methods are required to account for such variability. Surface features can protrude beyond the first or first few grid layers, whence the usual similarity theories (e.g., Monin-Obukhov) are invalid. The dependence of land-surface fluxes on synoptic flow also needs study. Wave radiation is ubiquitous in mountain terrain, and upper boundary conditions need to be designed accordingly.
- 3. Model Initiation: Data from a suite of platforms (surface, UAVs, balloons) can be assimilated into mesoscale models, for which new methodologies must be developed. Dense surface networks together with high-resolution grids may perform better, and profile data may be more effective than surface obs. Available data assimilation methods need to be evaluated for complex terrain. Methods of optimal sensor siting need to be developed and careful studies on initialization techniques including sensitivities to land-surface are required.
- 4. Small-scale Parameterizations: Representing processes operating at scales less than five grid increments is a fundamental problem. The processes are vital as they represent local processes, influenced by terrain, at the scale of small unit operations, and they can work together moving energy upscale. The primary parameterizations required are: a) Clouds their formation, maintenance, bases, tops, precipitation type and visibility restrictions; b) Turbulence the primary means of heat, mass and moisture exchange driving dust lofting, low cloud life cycles, and CBREN dispersion; c) Radiation the key to local heating and cooling near the surface is highly dependent on terrain, slope, local land surface, and clouds; d) Aerosols dust entrainment, visibility, cloud nuclei, modification of radiation; and e) Waves produced by flow over large and small complexities of terrain, modify the energy exchanges, create turbulence, and generate clouds but are poorly represented in current models.

**Impact:** The knowledge base gained through this fundamental research will benefit DoD operations (e.g. mountain warfare and operations in data-denied areas) by enabling: (i) improved prediction of environmental conditions at tactically-relevant scales, and (ii) improvement of DoD global and mesoscale NWP by eliminating a major source of forecast errors due to the improper treatment of atmosphere-terrain interaction processes.

**Research Topic Chiefs**: Dr. Ronald J. Ferek and CDR Daniel Eleuterio, Ph.D., Office of Naval Research, and Dr. Walter Bach, Army Research Office

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### **Bacterial or Cellular Controllers for Device Autonomy**

**Background:** Microbes and other cells possess sensory systems that interrogate their surrounding environments and then process and respond to this information. Stimuli known to provoke responses in microbes and cells include light; minerals; multiple bi-phasic interfaces (e.g., air/water or water/surface); temperature; salinity; specific chemical cues; mechanical stresses; and possibly acoustic impulses. Cellular responses include locomotion; or changes in cell membrane properties, colonization, metabolism or gene/ protein expression. With synthetic biology it has been possible to insert specific sensory, regulatory and response circuits into cells. For example, bacteria have been programmed to navigate along the edges of light fields<sup>1</sup>, to "count" using genetic timing circuits<sup>2</sup>, and to synchronize an oscillating cellular function<sup>3</sup>. It is of interest to see if bacteria or cells could be used as 'smart interfaces' or controllers for nonliving systems such as micro-robots

Cells have been used to process environmental information in certain types of biosensors to detect an analyte, and then generate a measurable optical or electrical signal. This MURI topic seeks to go beyond simple biosensing to using bacteria or cells to continually monitor the environment for multiple features of interest and then use this information to control a device. For example, a bacteria that chemotaxes toward an analyte could be coupled to a micro-robot and instruct it to move toward that analyte.

### **Objectives:**

To enhance understanding of microbial or cellular sensory and signal transduction pathways, to learn how to manipulate these for specific stimuli and responses, and to determine if these pathways can be connected through organic/inorganic interfaces to control an engineered device or system, such as a robot.

#### **Research Concentration Areas:**

Expertise in micro- and molecular biology, membrane biophysics, synthetic biology or bioengineering, material/interfacial science, opto-electronics, and/or signal processing is required to elucidate and manipulate microbial signal processing and transmission to a nonliving platform. Specific areas of interest include: (1) characterization of microbial/cellular (M/C) receptors for specific chemical cues and mechanisms of chemotaxis; (2) characterization of M/C sensing of non-chemical cues (e.g., vibration, sound, EM fields) and mechanisms of signal transduction; (3) novel materials to enable translation of M/C signals into external signals interpretable by a non-living platform (e.g., flagellar motion or other mechanical oscillations; optical, electrical or magnetic outputs); (4) signal processing (amplification and transduction) of M/C produced signals along with control algorithms to direct a device (e.g., robot) to carry out instructions; and (5) signal processing to enable feedback from a device to the M/C controller. Simple translation of external stimuli to an optical or electrical signal (as used in a biosensor) is not of interest unless the latter results in true control of an engineered device or system. Research focused on prosthetics or *in vivo* systems are also outside of the scope of this topic.

<sup>&</sup>lt;sup>1</sup> Tabor, J.J., Salis, H., Simpson, Z.B., Chevalier, A.A., Levskaya, A., Marcotte, E., Voigt, C.A. and Ellington, A. D. (2009) <u>Cell</u> **137(7)**: 1271-1281 <sup>2</sup> Friedland, A.E., Lu, T.K., Wang, X., Shi, D., Church, G., and Collins, J.J. (2009) <u>Science</u> **324**: 1199-1202

<sup>&</sup>lt;sup>3</sup> Danino, T., Mondragon-Palomin, O., Tsimring, L. and Hasty, J (2010) Nature **463**: 326-330

# Impact:

Enabling a living cell to interrogate an environment for multiple stimuli or features of interest, process this information and then convey a set of outputs or instructions to control a device will offer novel, smart interfaces for autonomous control. Success will depend on our ability to program cells to detect and process environmental information with minimal cross-talk, and then to convert cellular outputs into signals interpretable by and that provide actionable direction to a silicon- or organic-based device or system.

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# NanoScience based High-Speed Fabrication of Full Function Hybrid Flexible Electronic Systems

Background: This MURI topic will develop nano-manufacturing methods for continuous highrate production of full-function hybrid flexible electronic systems. Such a system will involve functional integration of organic, inorganic and biological materials on flexible substrates. Flexible electronic systems are stretchable, rollable and foldable, but they need to keep computing, sensing, powering and displaying. To achieve true flexibility and retain fullfunctionality, new materials and device architectures are needed that are built upon first principles molecular level design, that are attuned to the properties of interest at the higher scales and that lead to reliable manufacturability and durability. Nano-scale building blocks, such as, quantum dots and nanowires, and their growth and assembly via nano-scale processes, such as, nanolithography and self-organization, will make possible thin, multi-level flexible devices. For cost-effective production, continuous, reel-to-reel manufacturing platforms are needed. Devising nano-scale manufacturing methods for the accurate placement of device elements and production of integrated systems on flexible media moving at high speed will be a challenge that this MURI topic is designed to meet. A full-function flexible electronic system will consist of a set of thin film devices, such as, displays, lighting, photovoltaics, sensors, actuators and antennae, performing a set of desired functions. It will be interactive and energy-efficient. Such a technology will open new opportunities for multi-functional systems on conformal and deformable surfaces, opening new applications for Navy/DoD and new industries.

**Objectives:** The research objective is to develop the scientific basis for nano-scale materials and processes organized around the concepts of molecular design and molecular self-assembly for fabrication of full-function flexible electronic systems. In this context, the objective is to develop an understanding of how dissimilar nano-scale materials organize in three-dimensional space on a flexible substrate; interact physically, chemically and electronically; deform physically without loss of form and function; exchange and process information efficiently; and be reliably manufacturable over a large-area, at high-throughput and low cost.

Research Concentration Areas: (1) Materials discovery for low exciton binding energy and high electron mobility, among other material attributes, and good film-forming and printing properties needed for nano-scale processes. (2) Device design and development via hybridization of nano-scale organic, inorganic and biological species and corresponding interface engineering for high-efficiency device performance. (3) Development of reliable and affordable nano-manufacturing platforms with flexibility in materials and features. Explore accelerated self-assembly processes for patterning molecular monolayers for feature definition, and forming donor-acceptor pairs in devices. (4) First principles design, development and nano-scale processing of a family of elements such as circuits, interconnects, microchips, logic, memory, interface, etc. for a full-function flexible electronic system.

**Impact:** The development of a high-rate nano-manufacturing technology for full-function flexible electronic systems will impact many applications. For example, such systems will enable the integration of GPS, threat detection, health monitoring, and communication into a soldier's uniform or onto a UAV's wings, resulting in increased mobility and significant weight and cost

savings. Potential Navy/DoD applications are wearable electronics, flexible tape sensors, flexible solar cells for energy harvesting, flexible displays and RFID for communication. The high-throughput nano-manufacturing technology will also benefit other system-on-film applications such as fuel cell membrane-electrode-assembly.

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# **Atomic-Scale Interphases: Exploring New Material States**

**Background:** Diverse phenomena such as high temperature creep, corrosion, electron transport, fracture, fatigue, superplasticity, recrystallization, yielding, and embrittlement depend strongly on effects at homo-phase and hetero-phase interfaces. These interfaces are also important for diffusion phenomena as they provide pathways into or within a material that are orders of magnitude faster than through crystalline regions. Interfaces and the movement of atoms within an interface play a crucial role in determining bulk properties, transport and reactions, reliability and service lifetime of virtually all materials.

New states of matter have been discovered to exist at crystalline interfaces, which are neither completely amorphous nor fully crystalline. These three-dimensional interfaces, called atomicscale interphases, include grain boundaries and dissimilar phasal boundaries and range from sub-nanometer to 15 nm in width. Changes in bulk properties can lead to an evolution represented as transformational pathways in which reactions and kinetics are determined by local atomic re-arrangements (interphase conformations or configuration types) dictated by local rather than overall global equilibrium. This counters the traditional view of interfaces as planar, non-transformable two-dimensional defects whose properties depend mainly on the macroscopic interfacial degrees of freedom. Applying newly developed principles of thermodynamics, it is possible to transform one atomic scale interphase (interphase) to another interphase through the use of temperature, chemistry, pressure, etc. These interphases exhibit drastically different structure and transport kinetics (up to 100,000 times). Each interphase is expected to be stable over a range of compositions and temperatures. A specific type of grain boundary defined in terms of its macroscopic character (crystallographic misorientation and inclination) may display multiple distinct interphases under different conditions (for example, at different temperatures). Additionally, as the average grain size is reduced, the volume fraction of grain boundaries relative to grains increases dramatically thus in the nano-grain range.; decreasing the average grain size of materials offer additional opportunities to further explore the interphase character, composition, and structure as it relates to bulk material properties such as superplasiticity, hardness, and transport. Nanostructured ceramics have shown unique mechanical properties such as very high hardness, high fracture toughness, and super-plastic behavior in normally brittle ceramics. The experimental hardness was shown to be sensitive to the grain size and the fraction of the amorphous grain boundary phase. Atomic and mesoscale microstructural imaging can reconstruct the three-dimensional (3D) microstructures of solids to establish new concepts and establish a deeper understanding of the evolution of microstructures and the effects of interphases on materials properties. Determining which fundamental aspects of interphases (e.g. free volume, bond density, energy, bond strength, etc.) most greatly influence particular properties will provide a critical link between the atomic scale and bulk properties.

**Objective:** To explore atomic-scale interphases in a variety of materials in order to establish a fundamental scientific foundation to predict and create new materials with specific, tailorable materials properties.

**Research Concentration Areas:** Establishing the scientific base will require a multi-disciplinary team (materials science, mechanics, mathematics, thermodynamics and kinetics, expertise in 2D, 3D, and 4D atomistic computational simulations and ab-initio modeling, surface and interfacial science, statistical mechanics, molecular dynamics, non-equilibrium processing, atom-scale thermodynamic and kinetic computation with rigorous experimental validation, and advanced analytical characterization such as aberration-corrected transmission electron

microscopy, femtosecond or electron loss spectroscopy, 3-D atom probe tomography in a combined, highly coordinated experimental, computational, and theoretical effort. The research will cover a wide range of materials (alloy, ceramics and ceramic/alloy interfaces). Areas of interest include, but are not limited to, the following: (1) characterizing and identifying atomic structure of interphases in materials at grain boundaries and phase boundaries, (2) establishing quantitative structure-property relationships for interphases, (3) creating interphase diagrams, (4) establishing stability parameters of interphase configurations, (4) identifying the atomic to meso-scale structure of disordered and/or ordered interphase configurations as a function of grain size, (5) exploring non-equilibrium and meta-stability aspects of interphases and their transitions (6) utilizing 3D reconstruction and analysis of interphase structures to gain insight and understanding of bulk material property changes, (7) computing to describe grain boundary energetics to link quantifiable grain boundary parameters to predict interphase influence on bulk material properties, and (8) identifying and characterizing the interphase transport.

Impact: Establishing a fundamental scientific foundation would lead to: (1) eventually controlling, the atomistic processes involved in the transitional pathways when interfaces transition from one interphase to another because of composition and/or temperature change, (2) create new materials with tailored materials properties, (3) realize predictable nanofabrication processes by design. Fundamentally, this research will create the basic structure-property-processing-performance relationships that must be established for nanomaterials and nanostructures. Reliability of nanostructures will rely on 3D control of surface/interface composition/structure to minimize defects and enable subsequent processing (e.g., nanoscale planarization, polishing), and on the ability to remove and repair defects in nanofabricated structures. The integration of nanoparticle and nanomaterial synthesis with subsequent manufacturing steps and the consolidation and forming of nanostructures into macroscopic objects will be created through a combination of new and traditional manufacturing processes, bridging top-down and bottom-up approaches. Potential DOD applications include power and energy (fuel cell and battery component), high temperature materials (improved creep-resistant alloys and ceramics), corrosion-resistant materials, force protection (ductile ceramics, damage-tolerant alloys).

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#### Nanofabrication of Tunable 3D Nanotube Architectures

Background: Nanotubes are now extensively used in tailoring material properties. However, due to their one-dimensional properties and limited length, success in capturing their extraordinary characteristics in tailoring material properties to date has been limited. Nanofabrication of three-dimensional nanotube networks with nodal connectivity will provide an innovative framework for next generation materials design. Selective design and fabrication of three-dimensional, truss-like, nanotube networks will enable translating their exceptional one-dimensional properties into three-dimensions. More importantly, the design of 3D truss architectures will offer the unprecedented option of taking advantage of the enormous surface area to volume ratio for materials functionality and tunability. The nanotube sidewalls of the 3D truss will be available for functionalization for a wide variety of applications, ranging from ultra high capacity compact battery electrodes and fuel cells, to efficient materials with isotropic thermo-electro-mechanical properties. Recent advances in nanoscale modeling of 3D nanotube networks has greatly clarified the fundamental physics of the effects of the truss geometry, nodal connectivity, and atomistic architecture on their ultimate properties. However, viable nanofabrication approaches for these 3D truss architectures has not been realized.

**Objective:** The objective of this MURI is to understand fundamental principles behind the assembly and properties of three-dimensional tunable nanotube architectures. Realizing this objective will require a closely collaborative, multidisciplinary basic research effort to discover mechanisms for nanofabrication and molecular synthesis of novel architectures complimented by atomistic and molecular modeling, and nanoscale materials processing and characterization. This multidisciplinary effort will combine expertise from chemistry, physics, material science, nanoengineering, and mechanical and electrical engineering disciplines.

Research Concentration Areas: Suggested research areas include but are not limited to: (1) Theoretical Modeling: Utilizing the latest advances in computational techniques such as first principle (ab initio), Density Function Theory, atomistic molecular dynamics, and mesocale computational approaches for linking atomistic materials configuration to its 3D properties. (2) 3D nanotube truss fabrication: Conceiving nanofabrication processes and commensurate molecular synthetic mechanisms for assembling architectures. Multiple processing schemes, such as bottoms-up molecular construction via covalent bonding, catalyst nano patterning or nanotube self assembly can be explored for controlled 3D nanotube nodal connectivity. Consideration should be given to the control of molecular composition at the nanotube nodal joints to optimize the 3D properties and network rigidity. (3) Characterization: Development of nanoscale characterization techniques to quantify the nanotube joint performance, in particular electrical and thermal transmission characteristics, shear rigidity, etc. Development of nanoscale high fidelity materials testing protocols for correlating the experimental data with theoretical predictions.

**Impact:** 3D nanotube truss network architectures open up large surface area in threedimensions at the nano scale. This enormous surface area at the nanoscale is an enabling attribute to numerous applications, such as, fuel cell electrodes, efficient hydrogen storage, three-dimensionally tailored lightweight, thermal or electrical properties. The fundamental results from this MURI will enable future exploitation of the exceptional thermo-electromechanical properties of 3D nanoarchitectures and open up a new paradigm of nanostructured materials design and numerous research opportunities of DoD interest.

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# **Quantum Memories and Light-Matter Interfaces**

Background: Quantum Information Science (QIS) is a very active multidisciplinary field drawing upon theoretical and experimental physics, mathematics, computer science, engineering, and materials science. Its scope ranges from fundamental issues in quantum physics to prospective commercial exploitation by the communications and computing industries. In QIS, quantum principles are incorporated into information processing, yielding revolutionary new possibilities, such as ultra-secure communication through public channels, ability to solve efficiently computational problems that are classically intractable, and sensing and imaging capabilities that are beyond what is possible today with only classical resources. While a broad range of fundamental discoveries have been made in QIS in the past two decades, many scientific challenges remain open. For example, distribution of entanglement over long distances is crucial both for fundamental tests on quantum correlations, and for applications in, e.g., long-distance quantum communication, quantum computing, and metrology. A fundamental building block underlying most of the QIS-enabled capabilities is the reversible and efficient mapping of quantum states between light and matter and storing of such states — quantum memory. Significant progress has been made in recent years on increasing storage lifetimes, efficiency and fidelity of quantum memories in different physical implementations and with different protocols. However, significant effort is required to improve on these benchmarks for the above-mentioned capabilities, and to combine them in one set-up.

**Objective**: The goal of this MURI is to demonstrate long-lived, high-fidelity quantum memories and efficient quantum interfaces between the memory ("stationary") and photonic ("flying") qubits. Possible implementations might include, but are not limited to, trapped ions or atoms, atomic ensembles, or solid state quantum bits for storage (e.g., spins in semiconductors, nitrogen-vacancy centers in diamond, or crystals doped with rare-earth atoms), all of which are coherently coupled to photonic qubits, preferably at telecommunication wavelengths.

Research Concentration Areas: Areas of interest include: (I) Developing quantum memories as specified below; and (II) Demonstrating protocols of interest with quantum memories and interfaces. (I) Desired characteristics of the quantum memories and interfaces are: long storage time (>1sec); high fidelity (>90%); high efficiency; multimode capacity; and, the ability to store and retrieve photons at telecommunication wavelengths. As many as possible of these characteristics are expected to be demonstrated in the same quantum memory. Theoretical protocols are sought to show where quantum memories with fidelity and efficiency at the level of 90-95% can help achieve goals impossible with classical interfaces. (II) The following demonstrations with built-in quantum memories are of interest: (1) Storage of non-classical correlations (e.g., entanglement) in a multi-photon quantum memory; (2) Entanglement between qubits stored in remote memories; (3) Entanglement swapping or teleportation; (4) Quantum error correction on the memory qubit for extended storage times; (5) Entanglement purification; (6) Loophole-free tests of Bell's inequality. (1)-(2) are the required demonstrations, and a subset of (3)-(6) is expected to be realized.

**Impact**: Quantum Information Science has a potential for revolutionary impact on many areas of physics, mathematics, and computer science with significant impact on the DoD mission relating to communications, computation, cyber security, and information assurance. For example, quantum communication offers the potential of ultra-secure communication not possible with

classical communication channels. Quantum computing offers the potential to break classical encryption methods and solve computational problems that are impossible to solve with classical computers. Quantum memory is one of the central elements toward achieving such capabilities.

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## **Biomolecule-Directed Assembly of Nanostructures**

Background: Recent developments in nanomaterials synthesis offer opportunities to understand the unique, controllable physical properties of nanostructures. This knowledge will allow these tunable materials to be used by creating complex, ordered multidimensional nanostructured architectures. Directed self assembly techniques that form ordered nanoscale arrays, specifically DNA- and peptide-based assembly strategies, offer a revolutionary means of creating these materials, as the entire assembly process is tunable and can be done in parallel fashion without the need for mechanical intervention. Biomolecules have a large degree of programmability, and conformations that are imparted via simple alterations in nucleotide or amino acid sequence, although currently we lack the knowledge to predict tertiary structure of many biomolecules. Ultimately developing the understanding to enable tunable, biotemplate systems capable of forming arrays will enable a renaissance of nanomaterials assembly research, such as precision, speed, programmability and versatility in materials design. The goals of this program are to develop the understanding of the factors that govern tertiary biomolecule structure and new self-assembly and other techniques to form versatile nanostructured arrays.

**Objectives:** Understand the specific, local interactions including: Van der Waals interactions, capillary forces,  $\pi - \pi$  binding, and hydrogen bonding that govern biomolecule tertiary structure, self assembly, and self repair. Exploit new nanostructured self-assembling materials that are capable of forming large-scale 1-, 2-, and 3-dimensional macro-scale arrays. Key goals for this research include: (1) The understanding and development of novel nanoscale ordering methods that are highly tunable and programmable in multiple dimensions and are capable to self repair so as to impart a large degree of versatility into assembly and biotemplating properties. (2) The formation of macro-scale materials with nanoscale ordering so as to create new materials with unprecedented photonic, electronic, magnetic, and physical properties that arise from the formation of ordered nanomaterial arrays.

Research Concentration Areas: Suggested research areas include researchers from the fields of nanotechnology, chemistry, biology, materials science and computational theory. Specifically, "bottom up" biomolecule-based assembly strategies with: (1) The development of new modeling techniques to understanding biomolecular folding and tertiary structure and how these effect self assembly and nanostructure, (2) The capability of forming large scale arrays that traverse the nanometer to millimeter length scales, and (3) Tunable lattice parameters and repeat distances of the resulting assemblies. Additionally, the development of an understanding of the factors that emergent properties of nanomaterial assemblies through empirical and computational methods will be crucial to the success of this research.

**Impact**: The ability to synthesize ordered nanometer-scale assemblies over millimeter-scale areas has potential to create a new generation of materials for incorporation into electronic and photonic devices. Nanomaterials possess unique electronic, magnetic, photonic and physical properties that are highly desirable for applications in miniaturized electronic and opto-electronic circuitry, high-density data storage and manipulation, and efficient energy harvesting and storage. Nanoscale ordering would allow for both maximum control over beneficial nanomaterial properties and integration of nanomaterials into future macroscale devices.

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# Nanostructural Control of Thermal and Electrical Transport Properties with Organic Hybrid Materials

Background: Most materials with high thermal transport properties tend to have high electrical transport properties and vice versa. Yet it is desirable to be able to control them independently for thermal management and energy harvesting applications. Materials with high electrical conductivity but low thermal conductivity are desirable for thermoelectric applications, while those with opposite properties would be good thermal conducting insulators for electronic applications. With most traditional materials the density and mobility of negative and positive charge carriers is interlinked with thermal transport and thermal power. It prevents independent control of electrical and thermal transport properties in such materials. The interplay, understanding and control of electronic, electrical and thermal properties pose daunting challenges spanning theory, simulation, materials synthesis and assembly. To control these properties independently will require controlling not only composition, but material architecture and assembly such that the electron and thermal transport are more strongly decoupled. A metamaterial approach may be necessary to manipulate these properties independently by decoupling electrical and phonon density of states, charge mobility and phonon group velocities, number of cold and hot electrons in conduction band, interfacial transport of electrons and phonons, etc. Recent interests of nanostructured hybrid organic materials and some reported experimental results showed that thermal and electrical properties can be influenced independently. Developing material building blocks to assemble into metamaterial assemblies such that electronic transport is described on a dimension different from traditional materials, while manipulating the structure and composition to control thermal conductivity, remains relatively unexplored. A dedicated multidisciplinary effort is needed to fully explore and create science fundamentals for such independent control. By properly controlling the nanostructural dimension, morphology and the energy levels between different materials at the interfaces, the overall structural properties may be tuned to exhibit different overall phonon transport and charge transport properties. Basic research is needed to exploit these concepts and in designing and preparing new materials that can decouple electron and thermal conductivity, that can alter their thermal and electronic properties in response to external stimuli, in developing theoretical insights to understand such phenomena outside of classical parabolic electronic band models, in developing techniques to measure thermal and electronic properties in situ and on individual components (e.g. nanoinclusions). This topic will be a collaborative research effort that tackles the problem from a combined perspective of material, thermal, material physics, and interfacial sciences. The research will exploit the phonon scattering properties of organics and the unique electrical conductivity of nanostructural materials in a hybrid organic/inorganic material to control these properties.

**Objective**: To investigate and understand how to control thermal and electrical transport properties in hybrid materials. It is of particular interest to manipulate these properties independently so that they fall in ranges that will make them attractive for thermal management applications. It is desirable to understand of the difference in behavior between bulk and nanostructures. Understanding of transport across interfaces is also important as a means to control the overall properties of the hybrid structures.

**Research Concentration Area:** Suggested research areas include but are not limited to: (1) theoretical understanding of transport behaviors of nanostructured materials, and across

nanostructured hybrid organic materials interfaces. (2) Material designs, synthesis and fabrication to test hypothesis and to exploit control of the transport properties. (3) Design experimental techniques to measure transport behavior at at various length scales including nanostructural scale and at their interfaces to aid in the understanding of the behavior, and to validate hypotheses.

**Impact:** This topic will provide the fundamental science base needed to address the thermal management and the energy harvesting required for future DoD systems. Advances in these areas will enhance performance of many systems that are limited by power or thermal loads. It will impact operations of the individual soldier to unmanned vehicles and space systems.

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# **Investigation of 3-D Hybrid Integration of CMOS/Nanoelectronic Circuits**

Background: Using three-dimensional (3-D) integrated circuits is a natural way to increase density and performance of advanced electronic systems because such circuits may provide very high bandwidth and low time delay ("latency") of component interconnects. However, the approaches explored until recently, including edge-wire bonding of chip stacks, and throughsilicon vias (TSV), cannot provide the interconnect density necessary for many advanced applications. Also, homogeneous chip stacks, with similar circuit architectures on each chip, face extremely challenging heat management problems. On the other hand, there has been substantial progress recently in the conceptual design of quasi-uniform nanoelectronic structures ("fabrics"), in particular those based on nanowire crossbars with novel cross-point devices and area-distributed interfaces, with a potential density up to 10<sup>12</sup> cm<sup>-2</sup>. There are very recent ideas on how such interfaces might be used to enable effective interconnects between layers of heterogeneous 3-D stacks without expensive nanoscale alignment of chips. Such a hybrid system would join traditional (CMOS) silicon transistor circuitry, with its high performance and design flexibility, to several high-density nanoelectronic layers connected with areadistributed interfaces, providing a 3-D interconnect fabric. This "nanofabric," while dissipating very low power, would provide an extremely high aggregate bandwidth and latency of interconnects, with an important option for system reconfiguration to increase defect tolerance and/or run-time adaptation.

**Objective**: To investigate and ultimately develop the key fundamental aspects of new approaches to 3-D integration of electronic integrated circuits, with ultrahigh performance at manageable power consumption.

#### **Research Concentration Areas:**

- (1) Experimental and theoretical development of novel 2 and 3-terminal crosspoint devices, including (but not necessarily limited to) nanowire field-effect transistors, and bistable /memristive two-terminal devices. Any devices with appropriate functionality, whose reproducible fabrication may be rationally envisioned, e.g., those based on organic and molecular layers, metal oxides, amorphous silicon, phase-change materials, etc., may be explored.
- (2) Theoretical and experimental study of floating-gate devices suitable for 3-D integration, including those based of thin-film transistors (TFT), band-engineered tunnel barriers, and new materials.
- (3) Design and experimental demonstration of nanoelectronic fabric and areadistributed interconnect topologies for realistic crosspoint devices which would match the desired system architecture, with due attention to the potential low cost and high yield of manufacturing.
- (4) Development of architectures and computer aided design of 3-D integrated circuits and systems on several levels of abstraction. For certain goals, not only digital, but also analog and mixed-signal versions, should be explored, with the option of integration of signal processing systems with multi-sensor chips, in particular focal-plane arrays.

To succeed, any research project within this topic needs to be based on a promising concept of 3-D integration. As a result, it will require a truly interdisciplinary effort by a multi-departmental team including experts in electron devices, materials, manufacturing, circuit architectures and electronic design automation, because any significant change in one aspect of

the desired 3-D circuit may require substantial modifications on other design levels.

**Impact:** Practical introduction of 3-D nanoelectronic integrated circuits would affect all areas of electronics, including terabit memories and high-performance logic and signal-processing circuits. Such progress would enable new ultra-compact, ultra-fast electronic sensing and signal processing systems that yield real-time results in incredibly small packages. Their impact on military command and control functions would be highly significant, while surveillance and communications also would be greatly enhanced.

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# Science of Cyber Security

**Background**: The security of DoD systems as well as civilian systems (systems of systems connected across large scale networks with rich connectivity between network domains including the internet) from a Cyber Security perspective has been a reactive technology effort, for the most part. As attackers invent new attacks, defenders develop defenses but the attackers are always ahead of the defenders. Most have come to believe this is a cycle that cannot be broken because these systems (the hardware, software, human user and the network that connects them) are too complicated to ever be modeled and their properties formally defined and verified. In fact no formal definition of Cyber Security directly related to the properties of such a system has been produced, let alone metrics devised that measure those properties.

**Objective:** This MURI's objective is to begin the development of an architecture or first principle foundation to define Cyber Security for such a system. The intent is to discover and define basic system properties that compose system security and other useful attributes, system properties that can be verified and validated through theoretical proof and/or experiment. The research concentration areas below represent one view of a potential architecture/foundation. Other views, such as network based views, are welcome.

Research Concentration Areas: The research may address any or all of the system components (the hardware, software, human user and the network that connects them). Areas of interest include but are not limited to defining formal logics for modeling the system, security policies, attacks, and defenses to allow discovery and analysis of basic system properties to do the following: (1) understand whether such a system can enforce those security policies in system components (2) and across components to understand security properties of the whole system (3) understand system capability, as defined in 1 and 2 above, against each class of attack, after defining classes of cyber security attacks that cover all known attacks (4) discover and formally define the effectiveness of cyber security policies and mechanisms (including defense, monitoring, responses, etc.) to those classes of attacks (5) formally define the adversarial process model with respect to the development of new classes of attacks (6) formally define metrics for basic system properties and system ability to enforce security policies and defend against classes of attacks (7) formally define other system properties and their metrics such as scalability, adaptability, ease of use, mission assurance, etc., so that potential system designs can be compared against these properties and the cyber security property. Impact: The development of the theoretical underpinnings (system properties and relationship to policies) and the theories and metrics (relationships between attacks, defenses, policies) will allow development methods to compare the Cyber Security and other properties of a system and consider the trade-offs among them for current and future systems. In addition, this research will enable the development of new technologies and supporting tools grounded on sound principles; it could help comparing capabilities among vendors of their technologies; it would encourage the creation of a new industry for security software engineering technologies; it will reduce costs by providing scientifically supported evidence of security properties rather than applying exhaustive testing to look for evidence of insecurity.

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## **Large Scale Integrated Hybrid Nanophotonics**

Background: In recent years great progress has been made in the field of nanophotonics. This trend is driven to no small part by the merging of photonics with nanoelectronics and the vision of chipscale optical networks. Unique waveguiding structures, such as slot and gap waveguides, as well as the exploitation of surface plasmon modes associated with metallic structures, or plasmons, allow for the unprecedented manipulation of light at sub-wavelength dimensions. Although a rich set of both passive and active nanophotonic components have been realized in both all optical and plasmonic formats, it is expected that the hybridization of these two technologies will lead to opportunities unattainable by each technology separately. Fundamental questions are bound to emerge in the largely unexplored field of hybrid nanophotonics. The development of this field will require new theories and computational tools to address the interaction of intense and rapidly varying fields with metals, semiconductor and organic materials operating in both linear and non-linear regimes. The development of novel near and far-field optical characterization tools will be needed to help answer fundamental questions and optimize device performance. By taking advantage of the best aspects of both technologies, new devices allowing for simultaneous electronic and optical functions can be realized. Such devices include new light sources, waveguides, antennas and detectors, frequency converters, modulators, quantum optical, and ultrafast optical components.

Hybrid nanophotonics will also require the development of novel nano-manufacturing techniques to facilitate the large scale deployment of the technology and to allow for its seamless integration with existing microelectronic/optoelectronic platforms. Although the recent emergence of deep UV CMOS fabrication has enabled a variety of Si based nanophotonic building blocks, the device performance with such deep UV processes can be severely impacted by the achievable minimum critical dimension and roughness associated with a typical commercial CMOS foundry. Hence, the fabrication of hybrid nanophotonic integrated circuits will require new high-throughput and large-area fabrication process with minimum post-fabrication component tuning. It is expected that advances in electron beam lithography, focused ion beam milling, nano-imprint lithography, or, to be determined bottom up approaches will be required. If successful, hybrid nanophotonic components could form the basis of a low-power, high-speed, lightweight optical technology that takes advantage of the tremendous synergy between semiconductor optoelectronics and plasmonics operating in the sub-wavelength regime.

**Objective:** Explore fundamental aspects of hybrid nanophotonic components and subsystems that capitalize on combining the complementary electronic and optical properties of metals and semiconductor nanostructures, and potentially the conducting oxide and organic regime. Implement design strategies for realizing integrated photonic waveguide networks and the associated active and passive components. Develop novel nano-manufacturing processes and designs unique to this area and that are scalable from the laboratory to industrial production. Implement computational, design and fabrication strategies for realizing a high level of hybrid nanophotonic functionality.

**Research Concentration Areas:** Areas of interest include, but are not limited to the following. (1) Novel material processing and fabrication techniques for realizing hybrid nanophotonics and its deployment in a large-scale, high-throughput format, (2) novel optical, plasmonic or hybrid

waveguide/interconnect structures designed to enhance evanescent and surface interactions, and the optimization of these structures for foundry fabrication; (3) hybrid nanophotonic components which capitalize on subwavelength optics as applied to detectors and sources and the related extreme light concentration, (4) hybrid optical and plasmonic cavity effects and their exploitation in novel devices, (5) hybrid structures and the efficient incorporation of non-linear materials to facilitate components and subsystems based on non-linear effects, (6) the integration of hybrid nanophotonics and an appropriate optoelectronic/microelectronic platform for the realization of higher levels of integrated functionality, and (7) characterization tools and computational and analytic design strategies for hybrid nanophotonics devices.

**Impact:** Hybrid nanophotonic devices will perform active optical functions that can impact a wide variety of sensing, security, communication and computing systems. Systems on a chip with unprecedented levels of integration, boasting digital/analog/power electronics plus optical interfaces, will become a reality. The integration of electronics and photonics will result in significant speed and power advantages and subsequent system improvements. Exploration into nanomanufacturing processes will lead to new opportunities and capabilities. On a more general level, the research in this new class of devices will allow for a deeper understanding of its ultimate capabilities and limitations.

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#### **Controlling the Abiotic/Biotic Interface**

Background: In recent years, many novel composite materials with unique physical and chemical properties have been created by incorporating biological molecules onto biological surfaces. The biological components impart functionality and reactivity to these materials, making them excellent candidates for use in sensors and biomedical implants, as well as reactive, self-healing, antimicrobial and smart materials. The properties of these composite and nanocomposite materials are established by the nature of the interface. Thus, the successful development of abiotic/biotic materials depends upon an ability to control the structure, reactivity, and local environment at the interface to achieve desired biological function. The abiotic/biotic interface presents unique challenges to surface science, as many biological systems require an aqueous environment to support optimal activity. However, advances in surface functionalization, immobilization, and patterning capabilities (e.g., nanolithography) for biological molecules enable increasingly sophisticated abiotic/biotic material synthesis. Moreover, highly developed surface-specific analytical techniques are now being used to interrogate biological samples (e.g., sum frequency generation (SFG) vibration spectroscopy and environmental scanning electron microscopy (ESEM)), and continuing development of these technologies now enables molecular and sub-molecular level measurements of liquid/solid interfacial environments with significantly enhanced sensitivity and resolution. In addition, advances in molecular simulation methods have improved capabilities for modeling hydration states of biological molecules in solution and on surfaces.

**Objectives:** The objective of this MURI is to develop a fundamental understanding of how the structure and activity of covalently immobilized peptides and/or proteins (natural, artificial, and those containing unnatural amino acids) are affected by the chemical and physical environment at the abiotic/biotic interface. Specific focus will be on understanding the effects of surface properties and the role of water at the interface on biological structure and activity, and tuning these effects to achieve desired biological function.

Research Concentration Areas: Suggested research areas may include, but are not limited to the following: 1) Determine the impact of changes in surface morphology/chemistry and the composition of the interfacial environment on the structure and activity of immobilized peptides/proteins. 2) Develop capabilities to model interactions between immobilized peptides/proteins and the surface, and between immobilized peptides/proteins themselves, in environments with varying levels of humidity and as a function of surface properties. 3) Modify surface/interface properties and/or composition to improve sequestration of water molecules at the interface and/or to mimic the natural aqueous environment of peptides/proteins. 4) Model and synthesize surfaces to promote predicted biological function through precise control of binding, conformation, and patterning. 5) Determine the impact of varying hydration levels (e.g., monolayer vs. bulk water) on the stability of immobilized peptide/protein structure and function and on the robustness of abiotic/biotic materials over time.

**Impact:** The research targeted in this topic will lead to a fundamental understanding of the properties that control the abiotic/biotic interface and the ability to manipulate properties at the nanoscale to produce desired activity. The ability to design surface properties and the composition of the interfacial environment to promote biocompatibility is critical for the successful incorporation of abiotic/biotic materials in applications of interest, including sensing,

catalysis, coatings, drug delivery, prosthetics, and biofilms.

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#### **Quantum Stochastics and Control**

**Background:** Controlling the dynamics of quantum systems via the manipulation of external parameters and/or measurement is an important phenomenon that lies at the heart of several fields including atomic and optical physics, chemistry, and quantum information. This need, coupled with recent advances in understanding and applications, have made quantum control theory a rapidly growing research field. Open-loop control techniques for closed quantum systems originated and evolved from quantum chemistry, and have had applications in diverse fields, from optics to quantum computing. On the other hand, with the advent of modern methods for probing and measuring quantum systems it became possible to consider closedloop control, and such research, especially for open quantum systems, has just begun. Although closed-loop control in general (classically) yields far better results for optimizing a chosen objective functional, many great challenges lie ahead because: 1) probing and/or interacting with external systems causes back-action, that destroys the quantum evolution; 2) the presence of quantum noise greatly complicates the notion of closed-loop control in quantum contexts; 3) additional complications arise due to the presence of delays in observation and computation that are larger than the times involved in the system dynamics. To optimize the controlled quantum systems, one must continually improve an estimate of the evolving system state through real-time measurements as one tries to control it. Unfortunately, current research reveals that classical stochastic control theory and approaches are not applicable to feedback control of open quantum systems. In an attempt to seek solutions, quantum stochastic analysis for quantum Master equations and quantum filtering for state estimation have begun to emerge. These provide the first steps towards a formal and unifying framework for the development of a new theory and techniques. A concerted research effort is urgently needed to enable systematic development of a general quantum control theory that is applicable to quantum systems in both Markovian and non-Markovian environments. It is anticipated that the theory and techniques developed will impact and enable the rapidly growing applications in quantum computing, quantum communications, quantum chemistry, quantum metrology, quantum sensing, and quantum imaging, among others that exploit quantum phenomena for revolutionary new capabilities in nano-technology.

**Objectives:** Develop a new mathematical theory unifying quantum probability and quantum physics, for the control of open quantum systems, in order to enable a toolbox of techniques and strategies applicable across a wide range of disciplines that seek to exploit quantum phenomena for revolutionary advances in capability.

Research Concentration Areas: Research concentration areas may include but are not limited to (1) Mathematical theory, analysis and techniques for quantum control problems abstracted from systems in quantum physics and chemistry; (2) Memory and other non-Markovian effects of the environment; (3) Quantum stochastic calculus for infinite-dimensional systems; (4) Connections between quantum control for Markovian and non-Markovian systems; (5) Computation schemes for quantum optimal feedback control; and (6) Experimental verification and simulation of quantum control techniques and strategies developed.

**Impact:** The proposed work will unify the fields of quantum probability, quantum physics, and quantum chemistry, to enable control and manipulation of quantum systems needed for any future "quantum engineering." The results of this research will enable development of

revolutionary quantum devices that are important for future military operations.

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# **Qubit Enabled Imaging, Sensing & Metrology**

**Background:** Motivated by potential revolutionary impact on computing and communications. quantum information processing has advanced in many ways since its effective creation in the mid 1990's. Qubits (two-level quantum systems) have proved to be a powerful abstraction in the development of quantum computation. The abstraction has been central to the development of physical implementations, analytical tools, and algorithms. Error-correction and decoherence mitigation strategies are also dependent on the concept of a qubit. Recently, the totality of these ideas has demonstrated unprecedented precision in atomic clocks and overcome severe robustness and precision challenges in neutron interferometers. Separately, very low power imaging systems have been proposed by exploiting qubit entanglement. Theoretical efforts have explored and discovered valuable properties of multi-gubit quantum states (Eq., GHZ and N00N states) that enable one to beat classical limits in measurement. Algorithms based on gubits and quantum circuits have been developed for phase estimation that overcomes classical shot noise limits. In addition, the quantum computing circuit paradigm of initialization (state preparation), processing (circuit), and readout provides a potentially powerful basis for QuISM. In one envisaged QuISM paradigm, a multi-qubit measurement probe or sensor head would be followed by quantum circuit operations and readout to provide an output superior to an entirely classical circuit. Other variations and refinements are possible.

**Objective**: The objective of this MURI is to explore, develop, and demonstrate multi-qubit systems to enable beyond classical capabilities in imaging, sensing, and metrology. Included in this objective are the discovery, exploration, and efficient preparation of multi-qubit quantum states advantageous for imaging, sensing, and metrology, processing circuits for these states to enable beyond classical capabilities, and readout to provide the required output. Exploitation of quantum correlations for remote sensing using photons is not a primary objective of this topic.

Research Concentration Areas: Work should advantageously exploit techniques developed for quantum computing and communications to enable the new capabilities for imaging, sensing, and metrology. Such techniques include, but are not limited to logic gates and circuits for measurement processing, qubit encodings, decoherence mitigation, and error correction. Some research concentration areas for this topic are: (1) theory to explore multi-qubit quantum states useful for beyond classical capabilities; (2) quantitative assessment of capabilities and comparison to classical systems; (3) efficient state preparation; (4) quantum circuits for processing these states; (4) readout techniques; (5) decoherence mitigation and error-correction for improved performance; (6) supporting algorithms as a basis for processing circuits; (7) connections between the solution of hard computational problems and overcoming classical limitations in imaging, sensing, and metrology; (8) entanglement as a resource; (9) suitable physical systems and key demonstration experiments. Physical systems of interests include trapped ions, atomic systems, superconductors, semiconductors, and photons.

**Impact**: Research successes here could enable beyond classical systems capabilities in a broad range of DoD applications involving imaging, sensing, and metrology. New revolutionary capabilities can be expected in time-keeping, magnetometry, gradiometry, super-resolution imaging, low power imaging, target discrimination, as examples. These provide superior core capabilities for the Army, the broader DoD, health care, and other commercial applications. Any step change in these core capabilities can be anticipated to have a profound impact.

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#### Flex-Activated Materials

Background: Bulk material properties and performance are predominantly derived from the material interfaces, inhomogeneities, and defects that comprise them. Historically, material property enhancements have been pursued from the strategy of engineering these features to restrict material response (including defect-free crystals to eliminate electrical and mechanical property degradation and fillers and fiber sizing to limit stress concentrations), and to provide unique "mixed" properties (such as toughened materials by mixing ductile filler particles into a brittle matrix material, hierarchical materials, and multifunctional materials). What has yet to be achieved is an approach to fabricating and designing material interfaces that enhances or replenishes macroscopic material properties as a result of mechanical deformation generated from common loads and use. In this new approach, the interface is between a material and a stress-activated molecular "additive." These interfaces will be incorporated into tailored molecular architectures to enable regio-selective activation, leading to enhanced macroscopic properties. Rather than considering mechanical deformation as another possible source of property degradation, this topic seeks to utilize mechanical energy, applied in the form of elastic (or recoverable) deformation, as a means to replenish and enhance a material's properties of interest. Recent first-ever demonstrations of stress-driven chemical reactions and the discovery of new theories and algorithms to efficiently solve first principles molecular dynamics problems provide a tremendous opportunity to establish a new paradigm in materials design and fabrication of bulk materials from nanoscale designs. This MURI seeks to provide the foundation for the molecular design of materials with stress-activated reactions that can be selectively activated within precise regions to enhance macroscopic material properties.

**Objective:** This MURI program will bring chemistry, manufacturing science, materials science, and mechanical engineering together to generate materials with stress-activated molecules that enhance macroscopic properties of interest when elastic force is applied. This will be accomplished by using computation to design stress-activated molecules and fabrication and theory to incorporate them into materials that demonstrate regio-selective enhancements.

Research Concentration Areas: Suggested research areas may include, but are not limited to the following: (1) Use computation and modeling to design reversible or irreversible stress-activated molecules, determine the most advantageous approaches for incorporating them into materials and predict the response of the molecule as a function of stress, material architecture, and molecular orientation. (2) Synthesize promising stress-activated molecules and incorporate them into material systems using nano- and molecular- scale manufacturing and generate molecular architectures that facilitate the activation of chemical reactions with a very high degree of geometric, topological, and orientation specificity. (3) Fabricate and characterize the macroscopic response of flex-activated materials to recoverable deformation, correlate to the molecular level, and demonstrate significant enhancement in macroscopic properties of interest.

**Impact:** This topic will generate new science and engineering concepts based on nanostructured materials that will have a wide variety of long-term uses within DoD. Proposers should identify relevance to a small subset of potential DoD interests, which include but are not limited to, variably permeable parachute materials, biodegradable packaging materials, coatings with properties that are enhanced with time, including chemical agent resistant coatings (CARC)

and coatings for rotorcraft blades, adaptable adhesives, battery and electrode reconfiguration for extended life, and barrier and transport membranes.

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# **Game Theory for Adversarial Behavior**

Background: Game theory, the formalized study of strategy, began in the 1940s by asking how emotionless geniuses should play games, but ignored how average people with emotions and limited foresight play; furthermore, how people under various cultural, social, and economic backgrounds will actually play games has not been taken into account. Consequently, traditional game theory is inadequate for modeling and analyzing strategic interactions including bargaining, games of bluffing, psychological impact of 9/11-style terrorist acts, and building up reputations for trustworthiness or ruthlessness in real life. A second aspect of Game Theory, in its purest form, is that the idealized notion of Nash equilibrium is impractical to use in practice (i.e., of non-polynomial complexity). Finally, it is questionable whether the oft-used notion of equilibrium in a repeated game is even relevant in situations where the adversary expects to score big psychological gains by a single large attack (e.g., IEDs or 9/11-style attacks). Despite these shortcomings, a game theoretic approach has, for example, the great advantage of allowing a modeler to capture succinctly the conflict inherent in dealing with an adversary, whose behavior we seek to reason about. Therefore, a new mathematical game theory in the context of behavioral and social sciences needs to be developed in a multi-disciplinary manner by combining tools and ideas from (to name a few) applied mathematics, statistics, political science, psychology, anthropology, cognitive science, evolutionary biology and computer science. Recent work on generalized Stackelberg games with applications to Home Security (as in LAX airport) and recent (successful) experiments conducted to study how networked groups make decisions (under partial information and competition) suggest that a multi-disciplinary approach to develop a game theory for adversarial behavior might succeed.

**Objective**: A new approach is sought on pragmatic aspects of Game Theory that would allow messy real-world situations to be modeled and reasoned about in a scalable fashion. Furthermore, the new theory should take human behaviors/characteristics such as reciprocity, limited strategizing, deception, learning, and interactions into account, and should be able to deal with inconsistent/ incomplete game state information.

Research Concentration Areas: Areas of research include, but are not limited to, (1) modeling of deception, reciprocity, limited strategizing, learning, and interactions in the context of game theory, (2) social evolutionary analysis of cultural mores (e.g. Pashtunwali) that could lead to formalization of cultural values and mathematical analysis of asymmetric information and various optimization objectives that are relevant to different cultural backgrounds; (3) generalizations of multiplayer game theory to handle imperfect information, dynamic group formation, deception, flexible/changing and hidden objectives of opponents, (4) characterization and development of algorithms for the value function of the games based on item (3); (5) characterization and analysis of differential value of the asymmetric information possessed by the adversarial entities; and (6) scalable, perhaps approximate, algorithmic techniques that could be used to assess implications of decisions.

**Impact**: Game Theory is a central tool in war-gaming and war-planning. Therefore, a new game theoretic approach that is capable of incorporating non-rational strategies will enable U.S. defense forces to better anticipate adversarial behavior. Furthermore, it will enable defense forces and humanitarian agencies to optimize the deployment of resources based on host nation sensitivities and biases. Advances that make Game Theory practical and relevant for

analyzing asymmetrical wars are likely to have a big impact on DoD.

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# **Light Filamentation**

**Background:** A light filament is a novel form of propagating energy that is a combination of a laser beam and plasma. Such a beam has three characteristics that make it unlike any other form of energy, and also make it ideal for remote detection of trace materials. First, like laser light, it is coherent. Second, unlike laser light, as the beam propagates it undergoes wavelength dispersion, creating a coherent beam with wavelengths across the entire visible spectrum. Since the beam contains laser radiation at every wavelength, it is sometimes called a super-continuum or white laser. The continuum has a high UV content, which makes it of interest for remote chemical spectroscopy. Third, beating the diffraction limit, it does not diverge in space. Unlike any other form of energy propagation, the light filament can be as small at a distant target as it was when it was created. Light filaments are formed when intense laser pulses are focused down, due to the nonlinearity of the air (the Kerr effect), to about 100 microns. At this point, the intense field ionizes the nitrogen and oxygen, creating plasma. The plasma stops the self-focusing, and equilibrium is reached. The complex interaction of the plasma and electromagnetic field creates the effects stated above.

These properties make the light filament ideal for detecting trace elements at standoff distances; their coherence and continuum of wavelengths, coupled with high intensity on the target (due to its small spot size) are perfect for spectroscopic analysis. At the same time the interaction of the plasma filament itself with a target material can be used for a remote plasma breakdown spectroscopy. The two simultaneous spectroscopic phenomena provide a unique remote ability for measuring molecular as well as atomic target information. Recently new phenomena have been discovered. When they are allowed to strike a plastic/polymer type surface, they create a broadband radio frequency pulse essentially, a local EMP that can be used to jam electronics. Moreover, for droplet-sized particles in clouds, it has been discovered that light filaments can propagate around a particle and re-form. This may have applications to imaging through clouds, an abiding battlefield problem. Other phenomena include radiation of millimeter and terahertz frequencies perpendicular to the filament; the demonstrated ability of the filament to guide electrical pulses, currents, and lightning; bright optical radiation perpendicular to the filament; the guiding of high energy, nano-second optical pulses; and the creation of multiple filaments for directed energy. These filaments are extremely rich in phenomena for potential applications, but the complex interaction of optical, plasma, electromagnetic concepts are poorly understood.

**Objective:** This MURI is not focused on the many potential applications. Instead its objective is to establish the underlying qualitative and quantitative understanding of the physical phenomena associated with optical filaments in order to create and control them, and in particular, to learn how to control bifurcation of the filament, how to predict its propagation length, how it interacts with matter, how to steer the filament, how to combine or raster filaments, the physics of the electromagnetic interactions, how to increase the energy carrying capacity of a filament, how to create and control multiple filaments, and how to direct various sources of energy over the filament.

**Research Concentration Areas:** Success in meeting the research objective will require interdisciplinary expertise from the fields of plasma physics, optics, electromagnetics, electro-optics, electronics, and numerical analysis. Suggested issues to be addressed include the control of the bifurcation of the filament, the prediction of its propagation characteristics and length, its interaction with matter, the steering of the filament, the combination or rastering of the filaments, the physics of the electromagnetic interactions, the physical modeling of atmospheric filament propagation based on

filament propagation within solid crystals, the energy carrying capacity of the filament, the creation and control of multiple filaments, the formation and control of arrays of filaments, the direction of electrical and optical energy within the filaments, the associated radiation from the filaments, the EMP caused by interaction of the filaments with matter, and the ability to image through obscurants. In addition, there may be new phenomena discovered in these highly complex processes.

**Impact:** Controllable light filaments could revolutionize remote detection, creating a new ability in standoff spectroscopic detection. Moreover, the possibility of imaging through clouds and other obscurants may solve an age-old battlefield problem. The phenomena offer the potential for a variety of directed energy applications.

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# **Novel Free-Standing 2D Crystalline Materials (Oxides/Nitrides)**

Background: Initial experimental studies and preliminary theoretical models on ultra-thin oxide films show that ionic conductivity increases as the film thickness is reduced. From these results it can be expected that a few atomic layer thick free-standing 2D oxides, without a substrate interface, could improve conductivity even further. 2D nitrides such as BN are also of interest for wide bandgap semiconductor applications as evidence of UV lasing of h-BN single crystals was recently demonstrated. Recent ab initio density functional calculations show that an h-BN substrate can induce bandgap in graphene indicating that next generation nanocomposites consisting of both 2D nitrides and graphene with unique properties are possible. Free-standing 2D oxides/nitrides could also serve as a model system for understanding the edge effects. doping, defect generation, etc., providing a wealth of new basic understanding for developing next generation advanced materials. Since stable 1D nanotubes of BN, ZnO, and V<sub>2</sub>O<sub>5</sub> etc. are routinely grown, 2D nanosheets of oxides/ nitrides (the building blocks of 1D nanotubes) can be expected to be stable as well. Indeed, initial efforts indicate that small but stable 2D samples of BN and Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>5</sub> can be made by mechanical exfoliation. However, comprehensive understanding of 2D oxides/ nitrides and nanocomposites to identify promising materials with unique properties is lacking. Due to the ionic bonding in oxides, and multi-components present in these materials, they pose significant challenges to process them as compared to covalent graphene. However, these materials are expected to offer unique properties such as high ionic conductivity, high temperature stability, etc. for the applications where graphene alone cannot be used.

**Objective:** The objectives of this MURI are to develop a predictive theoretical framework to identify promising 2D free -standing crystalline oxides/ nitrides and nanocomposites, to innovate processing methods to consistently grow high quality large area 2D free -standing crystalline oxides/ nitrides, and to develop unique characterization techniques for conducting 2D materials research.

Research Concentration Areas: Suggested research areas may include but are not limited to the following: 1) Develop comprehensive theoretical models of free-standing 2D oxides/ nitrides and their nanocomposites, e.g. models to predict electronic structures of novel 2D nanosheets and bi-layers of similar or different materials 2) Investigate nucleation, growth and stability of 2D oxides/nitrides to develop innovative processing methods 3) Conduct experiments to understand the effects of defects and doping on the physical properties of free-standing 2D oxides, 2D nitrides and nanocomposites and 4) Processing of prototype devices utilizing novel 2D oxides/nitrides.

**Impact:** This MURI provides opportunities to develop novel materials with unique physical properties such as high ionic conductivity to make next generation devices and to use in thermal management. More specifically, this investment is expected to ultimately result in developing next generation bio- and chemical sensors, low power electronics, energy sources, DUV light emitters, multifunctional composites with better performance for military applications.

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Submit white papers and proposals to the Army Research Office

#### Value of Information for Distributed Data Fusion

Background: Shannon's information theory was developed to provide quantitative measures of data transmission over a noisy channel. Characterization of the information content and its value contained in the data were left unaddressed. Filling this gap is critical since a major challenge facing the current information explosion is the effective analysis, fusion, and exploitation of distributed data/information. Traditionally, data fusion is set up to passively fuse all received data. Such an approach is computationally challenging and operationally ineffective because improvements in information accuracy are not guaranteed. This issue can be addressed or alleviated by incorporating the information's value – the delta in measured performance with and without the information (relative to some objective metric). Key challenges are (1) the lack of understanding of how quality of information impacts the value of information, (2) the difficulties of characterizing the information content of data, and (3) the complexity of addressing the close coupling between the value of information and intended tasks. Value as a concept has different connotations in different disciplines. Research is needed to understand the different definitions and dimensions of value (e.g., in socio-cognitive and communications networks) and from that understanding to create a quantitative. mathematical value metric. Recently efforts in information evaluation such as source data characterization, actionable information formalism, and interactive sensing for fusion based on data evaluation, have made some progress, although these methods have been predominantly ad hoc. Regarding the specific area of fusion, preliminary studies using heuristic methods have indicated that incorporating the value of information can indeed improve overall performance. However, there currently is no theoretically founded rigorous approach to this problem – a requirement for advancing fusion performance in complex information systems.

**Objective:** Create a mathematical framework and computational methods for characterizing the value of information for distributed data/information fusion. Establish fundamental principles for automated information processing to address issues arising from collaborative sensing by teams of autonomous sensing systems as well as the integration of distributed datasets.

Research Concentration Areas: Suggested research areas may include, but are not limited to (1) Theory and associated metric(s) for characterizing the value of information: the impact of the value of information on object recognition and tracking, the relevance of features contained in the data. Approaches to quantitatively characterizing human's capability of assessing information value are of interest. Emphasis on EO/IR image/video data, acoustic and RF signals is desirable; (2) Approaches to determining quality of information metric objectives for distributed data fusion; (3) Methods for distributed data fusion based on the value of information. Quantitative tradeoff between the value of information and the cost of obtaining the information should be considered (e.g., under communications constraints). Of particularly interest are methods for the modeling and pricing of uncertainty of information in distributed data fusion; (4) A framework to determine the requisite information needs or the completeness of information that can achieve value for automated decision-making; and (5) Methods for adaptive learning of the value of information to support dynamic operations with evolving mission objectives.

**Impact:** Effort would advance research on information evaluation for distributed data and information processing, and enhance defense capabilities for intelligence analysis, command and control, and decision making. These capabilities are of critical importance to many military

applications including surveillance, reconnaissance, situational awareness, and autonomous systems. Civilian applications include information management and homeland security.

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